summer undergraduate research fellowship

SURF 2004

colloquium

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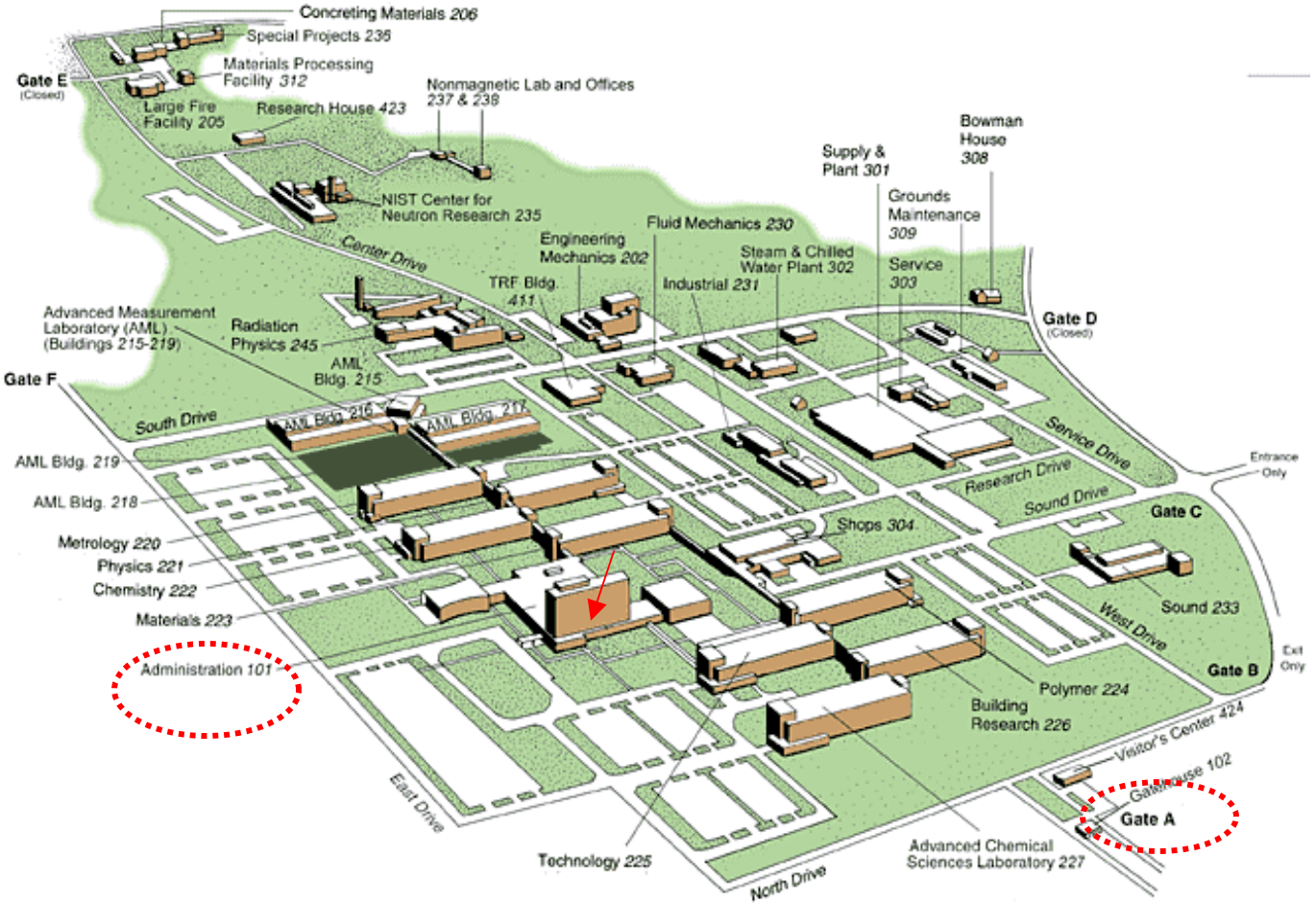

Enter through Gate A for Visitor Center security check in.

SURF Student Colloquium: Tuesday - August 10, 2004
Plenary Session: Green Auditorium, Administration Building (101)

TIME	SPEAKER	UNIVERSITY	TITLE	LAB
9:00A	Lisa Fronczek	NIST SURF Director	Welcome	MEL
Moderator: B. J. Yoblinski Appalachian State University				
9:10A	Ramsey Zeitoun	University of Maryland, College Park	Development of a Bismuth Filter for the Filter Analyzer Neutron Spectrometer	MSEL
9:40A	April Colleton	Rochester Institute of Technology	Electropolymerization and Functionalization of Polymeric Material for DNA Sensing in Microfluidic Channels	CSTL
10:10A	Stephanie Svetlik	Pomona College	Nanomechanical Properties of TiO_2/Epoxy Nanocomposites	BFRL
10:40A	Karolina A. Sarnowska	Mississippi State University	A Comparison of Contention Resolution Schemes for Optical Burst Switching Networks	ITL
11:10A	BREAK			
11:25A	Wei M. Tan	University of Colorado	Investigation of Carbon Contamination of CD Reference Materials	EEEL
11:55A	Kelly McQuighan	Rice University	Automation and Testing of a New Plastic Scintillator Dosimeter for Radioactive Sources Used in Prostate Cancer Brachytherapy	PL
12:25P	Jeffrey R. Comer	University of Akron	Fractional Kinetics in Atomic Force Microscope Assisted Oxidation of Zirconium Nitride	MEL
12:55P	LUNCH: SURF DIRECTORS AND SPECIAL GUESTS – EMPLOYEE LOUNGE			

SURF Student Colloquium: Tuesday - August 10, 2004
Parallel Sessions: Lecture Room A, Administration Building (101)

TIME	SPEAKER	UNIVERSITY	TITLE	LAB
Moderator: Albert Lee National Institute of Standards and Technology				
2:30P	Matthew A. Armstrong	Davidson College	The Effect of Temperature on the Fluorescence of Phycoerythrin and Oligonucleotide-Labeled Fluorophores	CSTL
2:50P	Brenna M. McGruder	Mississippi State University	Real-Time Measurements for Cancer Detection Using Telomerase	CSTL
3:10P	Felicia Tsai	Rensselaer Polytechnic Institute	Analysis of a Model Drug Delivery System Using Cluster Secondary Ion Mass Spectrometry (SIMS) and Trace Narcotics Detection Using Ion Mobility Spectrometry (IMS)	CSTL
3:30P	Claribel Acevedo-Velez	University of Puerto Rico, Mayaguez	Automation of the NIST Hydrometers Calibration Service	CSTL

SURF Student Colloquium: Tuesday - August 10, 2004
Parallel Sessions: Lecture Room B, Administration Building (101)

TIME	SPEAKER	UNIVERSITY	TITLE	LAB
Moderator: Rex Ramsier University of Akron				
2:30P	Ben Baumgold	Massachusetts Institute of Technology	Magnetic Refrigeration: Perfecting the Process	MSEL
2:50P	Constance P. Lee	Northwestern University	Grain Growth and Boundary Migration in Strontium Titanate	MSEL
3:10P	Robert Theodore Harris	University of North Carolina, Charlotte	Combinatorial Study of Nickel-Gold p-contacts for Blue InGaN Light Emitting Diodes Comparing Electron Beam and Pulsed Laser Deposition Techniques	MSEL
3:30P	Ileana Marquez Pazos	Barry University	Tenary Phase Diagram of the System Bi_2O_3-Fe_2O_3-Nb_2O_5	MSEL

SURF Student Colloquium: Tuesday - August 10, 2004
Parallel Sessions: Lecture Room C, Administration Building (101)

TIME	SPEAKER	UNIVERSITY	TITLE	LAB
Moderator: Javier Figueroa University of Puerto Rico				
2:30P	Ángel G. Fuentes-Figueroa	University of Puerto Rico, Mayaguez	Testing Software Packages for Gamma-Ray Spectrometry Measurements Using Germanium Detectors	PL
2:50P	Eric J. Montgomery	University of Maryland, Baltimore County	Exciting Frontiers in Single Photon Counting Detectors	PL
3:10P	Candace Pfefferkorn	Gettysburg College	Nanotube Formation from Biological Membranes Using Optical Tweezers	PL
3:30P	Jennifer Robinson	Cornell University	Improving Trapping and Detection of BECs in Optical Lattices	PL

SURF Student Colloquium: Wednesday - August 11, 2004
Parallel Session: Lecture Room A, Administration Building (101)

TIME	SPEAKER	UNIVERSITY	TITLE	LAB
Moderator: Ana Feliciano University of Puerto Rico				
9:00A	Angelica Perez-Andujar	University of Puerto Rico, Mayaguez	Test Report of Radiation Detectors Against the ANSI N42.32, N42.33, N42.34, and N42.35 Standards	PL
9:20A	Miguel A. Morales	University of Puerto Rico, Mayaguez	Phase Diagram of a Gas of Atomic Bosons, Atomic Fermions, and Heteronuclear Molecules	PL
9:40A	Thomas Cleveland	Tulane University	Using Neutron Imaging to Analyze the Internal Structure of Biological and Mechanical Objects	PL
10:00A	Katherine E. Myers	Lebanon Valley College	Dyamic Imaging of Lipid Bilayers on Chemically Modified Surfaces	PL
10:20A	BREAK			
Moderator: Robert Shepard Science and Engineering Alliance				
10:30A	Mikolaj Bykowski	Lehigh University	Evaluating the Fire Resistance of Structural Steel	MSEL
10:50A	Nathan J. Mesick	Rensselaer Polytechnic Institute	Diffusion in Nickel-Base Superalloys and Bond Coats	MSEL
11:10A	Alexander U. Adler	The Pennsylvania State University	Phase Equilibria Studies of Bi_2O_3-Mn_2O_3-Nb_2O_5	MSEL
11:30A	Cornelius Griggs	University of Maryland, College Park	Investigating Mechanical Properties of Thin Films	MSEL
11:50A	LUNCH			

SURF Student Colloquium: Wednesday - August 11, 2004
Parallel Session: Lecture Room A, Administration Building (101)

Moderator: Alonzo Ashley Stanford University				
1:30P	Alina Butler	Mississippi State University	Evaluation of Alpha Spectra Deconvolution: A Beam Piercing Through the Vail of Obscurity	PL
1:50P	Robert J. Radford	University of California, Santa Barbara	An Exploratory Data Analysis for Plutonium Contamination	PL
2:10P	Daphne Chang	Duke University	In Search of Higher Pu Sensitivity for TIMS	PL
2:30P	Paul Speicher	University of Virginia	Ionizing Radiation Dosimetry Using Water Calorimetry: The Exciting World of Water Temperature	PL

SURF Student Colloquium: Wednesday - August 11, 2004
Parallel Session: Lecture Room B, Administration Building (101)

TIME	SPEAKER	UNIVERSITY	TITLE	LAB
Moderator: Jeanice Brown Thomas National Institute of Standards and Technology				
9:00A	Jennifer L. Breidenich	Smith College	Investigating Interactions Between Colloidal Material and Polycyclic Aromatic Hydrocarbons: Quantifying Sorption Characteristics	CSTL
9:20A	G. Barratt Park	Davidson College	High-Temperature Unimolecular Isomerization Kinetics of 1,4-Pentadiene	CSTL
9:40A	Eric Shamay	California Polytechnic State University	Accessing Modern Real Fuels: Kinetic and Thermodynamic Property Databases	CSTL
10:00A	Kevin A.Wepasnick	Franklin and Marshall College	Web-based Databases for Chemical Properties	CSTL
10:20A	BREAK			
Moderator: David Ross National Institute of Standards and Technology				
10:30A	Kellie M. Smith	Mississippi State University	Determination of Folate Vitames in Spinach via Liquid Chromatography Combined with Ultraviolet and Fluorescence Detection	CSTL
10:50A	Stacey J. Hoebel	University of Wisconsin, Madison	Temperature Gradient Focusing	CSTL
11:10A	Tracy Stover	Murray State University	Compton Suppression for Neutron Activation Analysis Applications at the National Institute of Standards and Technology	CSTL
11:30A	Maria Santiago	Inter American University of Puerto Rico, San German	Advanced Inkjet Printing Technology for Trace Explosive Standards	CSTL
11:50A	LUNCH			

SURF Student Colloquium: Wednesday - August 11, 2004
Parallel Session: Lecture Room B, Administration Building (101)

Moderator: B. J. Yoblinski Appalachian State University				
1:30P	Alan A. Thrift	University of North Carolina, Charlotte	Mechanical Design of a Uniaxial Load Frame with High Load Capacity	MSEL
1:50P	Veronicz Rodriguez-Rivera	University of Puerto Rico, Mayaguez	Phase Behavior of Mixed Lipid Bilayered System	MSEL
2:10P	Teresa L. Jacques	Smith College	X-ray Reflectivity Study of the Formation of Alkane Films on OTS-coated Silicon Surfaces	MSEL
2:30	Jesse W. Hwang	University of Maryland, College Park	Development of Calcium Phosphate-gelatin Composites	MSEL

SURF Student Colloquium: Wednesday - August 11, 2004
Parallel Session: Lecture Room C, Administration Building (101)

TIME	SPEAKER	UNIVERSITY	TITLE	LAB
Moderator: Dimitrios Goulias University of Maryland				
9:00A	James E. Wells	Davidson College	The Design and Fabrication of a Thermally Driven Outdoor Sealant Tester	BFRL
9:20A	Dahlia Ashford	Mississippi State University	The Influence of Chemical and Environmental Factors on Measurements of the Degree of Hydration of Cement Pastes	BFRL
9:40A	Michelle N. Clarke	Johns Hopkins University	Characterization of the Microstructure and Properties of Fire Protective Materials	BFRL
10:00A	Dorea R. Ruggles	Gustavus Adolphus College	Database-assisted Design for Structures Subjected to Wind Loads	BFRL
10:20A	BREAK			
Moderator: Loretta Moore Jackson State University				
10:30A	Whitney B. Austin	Jackson State University	Tracker Calibration for Immersive Visualization in a Reconfigurable Automatic Virtual Environment	ITL
10:50A	Daniel S. Blanchard	Millersville University	Computer-Aided Camera Placement for Facial Recognition	ITL
11:10A	Debra Lauterbach	Iowa State University	Adding Speech to Text Transcription to a Video Annotation Tool	ITL
11:30A	Angel L. Villalain-Garcia	University of Puerto Rico	Authentication and Authorization in a Distributed Computer Server	ITL
11:50A	LUNCH			

SURF Student Colloquium: Wednesday - August 11, 2004
Parallel Session: Lecture Room C, Administration Building (101)

Moderator: Jeffrey Campbell University of Maryland, Baltimore County				
1:30P	William Ashley	University of San Diego	Verifying Deleted File Recovery Tools	ITL
1:50P	Michel Le	University of California, Irvine	Investigating Reliability Characteristics of Medium-Sized Service-Oriented Architecture	ITL
2:10P	Paul William Matthews	Coppin State University	Reducing NSRL Overhead: Finding Similar Attributes in Multiple Language Versions of Microwoft Windows' Internet Files	ITL
2:30	Shauntia Burley	Coppin State University	Creating 3D Visualizations for the NIST Digital Library of Mathematical Functions	ITL

SURF Student Colloquium: Wednesday - August 11, 2004
Parallel Session: Lecture Room D, Administration Building (101)

TIME	SPEAKER	UNIVERSITY	TITLE	LAB
Moderator: Sarah Gilbert National Institute of Standards and Technology				
9:00A	Anna Stelzenmuller	Southern Methodist University	Surface Treatment and Characterization of Ag/AgCl Micro-Reference Electrode Arrays for BioElectronics	EEEL
9:20A	Jennifer M. Lenkner	College of Mount St. Joseph	Development, Fabrication, and Characterization of Novel Electrodes for Use as Cell Based Sensors	EEEL
9:40A	Quenton Bonds	University of Alabama, Birmingham	The Study of Metal Work Functions by Measurement of Capacitance-voltage, Scanning Kelvin Probe Microscopy	EEEL
10:00A	Stephen Lin	University of Pennsylvania	Thermal Characterization of Microhotplate Devices and Gas-Sensor System-on-a-Chip (SoC)	EEEL
10:20A	BREAK			
Moderator: Rex Ramsier University of Akron				
10:30A	Amanda Frederick	Miami University	Use of a Laser Vibrometer for Measuring Spindle Error Motion	MEL
10:50A	Jonathan Lee	University of California, Berkeley	Eliminating Rotational Errors in C-AFM's 6-axis Stage	MEL
11:10A	Leah Pike	Washington University in St. Louis	Image Analysis of MEMS-Based Nanopositioning Stages	MEL
11:30A	David Walker	University of Rochester	A Standard Architecture for Naval Training Simulations	MEL
11:50A	LUNCH			

SURF Student Colloquium: Wednesday - August 11, 2004
Parallel Session: Lecture Room D, Administration Building (101)

Moderator: André W. Marshall University of Maryland				
1:30P	Jennifer L. Wiley	University of Maryland, College Park	Validation Experiments for the Fire Dynamics Simulator, Version 4.0	BFRL
1:50P	Andrew C. Milliken	University of Maryland, College Park	Wireless Telemery for Fire Research and Fire Service Applications	BFRL
2:10P	Ian P. Rafferty	St. Mary's College of Maryland	Flame Size vs. Heat Release Rates	BFRL
2:30P	Claire V. Lewinger	University of Florida	A Study of the Effect of Fire on Steel Framed Buildings	BFRL

SURF Student Colloquium: Thursday - August 12, 2004
Parallel Session: Lecture Room A, Administration Building (101)

TIME	SPEAKER	UNIVERSITY	TITLE	LAB
Moderator: David Tanenbaum Pomona College				
9:00A	Han Yong Ban	Pomona College	Lifetime Measurement of Erbium Transition $4f^{12}6s^2 \rightarrow 4f^{11}(^4I^{\circ}_{15/2})\,5d_{5/2}\,6s^2$	PL
9:20A	Jennifer Antonnen	Carnegie Mellon University	Determining Plasma Temperatures with Spectroscopic Data	PL
9:40A	Christopher J. Stanford	University of Southern California	Sub-millimeter Absorption Spectroscopy of Water Vapor	PL
10:00A	Alexander Fried	University of Pennsylvania	Digital Image Plate Diagnostics for Use in Ultraviolet Spectroscopy	PL
10:20A	BREAK			
10:30A	Samuel Brewer	Appalachian State University	Visible Imaging of Highly Charged Ion Clouds in the NIST EBIT	PL
10:50A	Andrew Schwarzkopf	Cornell University	Size-Dependent Optical Properties of Gold Nanotubes	PL
11:10A	Meeri N. Kim	Boston University	Searching for Evidence of Correlated Photons Formed by 4-Wave Mixing	PL
11:30A	LUNCH			
Moderator: Alonzo Ashley Stanford University				
1:30P	MacArthur Weatherspoon II	University of Cincinnati	Neutron Spectroscopy	PL
1:50P	Eric D. Kelsic	California Institute of Technology	Efficient Implementation of Error-Handling for Quantum Key Distribution	PL
2:10P	Matthew Davidson	Catholic University	Quantum Cellular Automat Architecture in an Optical Lattice	PL

SURF Student Colloquium: Thursday - August 12, 2004
Parallel Session: Lecture Room B, Administration Building (101)

TIME	SPEAKER	UNIVERSITY	TITLE	LAB
Moderator: Ana Feliciano University of Puerto Rico				
9:00A	Charles Brooks	University of Maryland, College Park	The Observance and Removal of PSS Top Layer in Poly(3,4-ethylenedioxythiophene)-polystyrenesulfonic Acid (PEDOT0_SS) Conducting Thin Films	MSEL
9:20A	Bryan I. Nishimoto	University of California, Irvine	Method Development for the Preparation and Analysis of Polymer Samples Using MALDI-TOF Mass Spectrometry	MSEL
9:40A	William J. Goodrum, Jr.	University of Virginia	Microfluidic Interfacial Tension Measurements: Getting the Most From Your Soaps	MSEL
10:00A	Nicholas R. Hughes	Southern Methodist University	Chaotic Mixing in Microfluidic Devices	MSEL
10:20A	BREAK			
Moderator: Chiara Ferraris National Institute of Standards and Technology				
10:30A	Stephanie E. Goldfarb	Cornell University	Factors Influencing the Determination of the Strain Energy Release Rate of an Adhesive Tape	BFRL
10:50A	Caitlin Baum	University of Maryland, Baltimore County	Characterizing Polymer Nanocomposites During Processing	BFRL
11:10A	Lloyd W. Gewuerz	Binghamton University, SUNY	The Capabilities of FDS for Prediction of the Steady-State Burning of Small-Scale Materials	BFRL
11:30A	LUNCH			

SURF Student Colloquium: Thursday - August 12, 2004
Parallel Session: Lecture Room B, Administration Building (101)

Moderator: James Batteas National Institute of Standards and Technology				
1:30P	Carmen Reedy	Radford University	Investigations of Explosive Particles in Simulated Fingerprints	CSTL
1:50P	Carolyn A. Kitchens	Appalachian State University	Preparation and Characterization of Proteins and Hybrid Lipid Bilayers on Gold Surfaces	CSTL
2:10P	Nathan T. Fisher	University of Maryland, College Park	Correlating HMDS (Hexamethyldisilazane) Modified Silica Substrate Surface Characteristics to Thin Film Morphology of Poly(3-hexylthiophene)	MSEL
2:30P	Brad R. Conrad	Rochester Institute of Technology	Time Domain Dielectric Spectroscopy Analysis of the Amorphous Phase in Semicrystaline Polycarbonate	MSEL

SURF Student Colloquium: Thursday - August 12, 2004
Parallel Session: Lecture Room C, Administration Building (101)

TIME	SPEAKER	UNIVERSITY	TITLE	LAB
Moderator: Raynett Prevo Alabama State University				
9:00A	Chris S. Garber	Austin Peay State University	Forensic Ballistics: Checking the Performance of Integrated Ballistics Systems with the Standard Bullet and Casing Project	EEEL
9:20A	Jessica Naff	Appalachian State University	Re-creation of Accelerant Burn Patterns on Carpet Using the Fire Dynamics Simulator	P
9:40A	Brian J. Simonds	Illinois Wesleyan University	Creating a Nanocapacitor to Measure the Energetics of Molecules in Self-Assembled Monolayers	EEEL
10:00A	Andrew Q. Chereck	Illinois Wesleyan University	Controlling a Johnson Junction Array with LabView	EEEL
10:20A	BREAK			
Moderator: Dan Rudolph University of Maryland				
10:30A	Dyami H. Jenkins	University of Maryland, College Park	Augmentation of the Statistical Test Suite for Random Number Generators	ITL
10:50A	Brendan Farrar-Foley	The George Washington University	PDA Forensic Tools: Overview and Analysis	ITL
11:10A	Soren Johnson	Boston University	An Intrusion Detection System in a Wireless Ad Hoc Network	ITL
11:30A	Jingsi Gao	Delaware State University	Wireless Enhancement for Storage Networking	ITL
11:50A	LUNCH			

SURF Student Colloquium: Thursday - August 12, 2004
Parallel Session: Lecture Room C, Administration Building (101)

Moderator: Larry Reeker National Institute of Standards and Technology				
1:30P	Van Molino	Princeton University	Markov Chains and MCMC Methods	ITL
1:50P	Brian G. Cordes	Worcester Polytechnic Institute	Developing a Graphical Tool to Determine the Estimation Capacity of an Experimental Design	ITL
2:10P	Michael Huber	American University	Streamlining the Production of Viewpoints in VRML	ITL
2:30P	Daniel A. Cogut	College of William and Mary	Fusion of Biometric Algorithms	ITL

SURF Student Colloquium: Special Presentations

DATE	SPEAKER	UNIVERSITY	TITLE	LAB
July 30	Alan Skaggs	Southern Methodist University	Cutting Forces in Aluminum Alloys	MEL
August 6	Dustin Diez	Rhodes College	Calibration of a Micro Force Sensors for the Characterization of Compliant Mechanism MEMS	MEL
August 6	Firouzeh Jalilian	University of Maryland, College Park	Developing a Graphical User Interface for the Mass Calibration Program	ITL

SURF STUDENT

Farewell Party!

Farewell Party

12:30PM

Friday, August 13, 2004

Farewell Party

Employees' Lounge

SURF STUDENT 2004

Abstracts

(Alphabetical by Student)

SURF Student Colloquium

NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Claribel Acevedo-Vélez	**Grant Number:** 70NANB4H1046
Academic Institution: University of Puerto Rico – Mayaguez Campus	**Major:** Chemical Engineering
Academic Standing as of September '04: Senior	
Current Career Plans: Plan to go to graduate school to pursue studies in Biomedical Engineering	
NIST Laboratory, Division and Group: Chemical Science and Technology Laboratory, Process Measurements Division, Fluid Flow Group	
NIST Research Advisor: Dr. Pedro Espina	
Title of Talk: Automation of the NIST Hydrometers Calibration Service	

Abstract of Talk:

A hydrometer is an instrument used to measure the density of liquids and other density dependant properties (e.g., specific gravity, proof spirit for alcohol solutions, API degrees for liquid petroleum products, and degrees Baume). The instrument consists of a sealed glass bulb with a thin graduated neck. When the instrument is placed in a liquid, its bulb portion submerges while the neck remains above the liquid surface. The length of neck floating over the liquid surface is directly proportional to the density of the liquid.

Currently, NIST calibrates hydrometers gravimetrically by measuring the buoyancy of the instrument when a specific neck scale-mark is aligned with the horizontal plane of a reference liquid. This calibration, which requires multiple observations of mass, temperature, pressure, and meniscus position, is done at 3 points, at approximately 10%, 50%, and 90% of the scale. The manual process is lengthy, tedious, and prone to operator errors.

This project seeks to automate the calibration method for hydrometers by controlling the gravimetric calibration system, with different types of hardware, using National Instruments LabVIEW. The improved performance of the automated method will be compared to that of the manual method using results of calibrations for various control hydrometers.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Alexander U. Adler	**Grant Number:** 70NANB4H1033
Academic Institution: The Pennsylvania State University	**Major:** Materials Science & Engineering
Academic Standing as of September '04: Sophomore	
Current Career Plans: To go to graduate school and study more about Materials Science.	
NIST Laboratory, Division and Group: Materials Science and Engineering Laboratory, Ceramics Division, Data and Standards Technology Group	
NIST Research Advisor: Dr. Terrell Vanderah and Dr. Michael Lufaso	
Title of Talk: Phase Equilibria Studies of Bi_2O_3-Mn_2O_3-Nb_2O_5	

Abstract of Talk:

Research on the Bi_2O_3-Mn_2O_3-Nb_2O_5 ternary system has many ramifications for those interested in the electric and magnetic properties ceramics can offer. Through X-Ray diffraction pattern analysis, applications of solid state chemistry, and existing knowledge of binary phase diagrams, we have constructed a phase diagram for this system that shows a few interesting caveats. In conjunction with the Metallurgy Division and TCI Ceramics, Inc., we have examined key compounds and mixtures involving these three compounds for their electric and magnetic properties in hopes of determining useful characteristics for industry such as their dielectric and magnetic properties.

Through carefully chosen points on the ternary plot between Bi_2O_3, Mn_2O_3 and Nb_2O_5 and the analysis of X-ray diffraction patterns of the said equilibrated compounds and solutions, we are able to map out single, double and triple phase regions. The "map" we create can be used by industry to generate compounds with specific qualities or perhaps realize that such compounds or qualities cannot be obtained through work with these three compounds; either way, saving a lot of time.

Enhanced knowledge in the area of "multiferroic" (materials blending ferroelectric and ferromagnetic properties) materials is key to technological progress in the future as such understanding may improve quantum computing, electronic circuits and wireless technology to name just a few areas. Through analyzing the applications and results of our system and covering the basic applications and findings of other such systems, I hope to present a well-rounded view of this field of research and its ramifications on the future of technology.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Jennifer Anttonen	**Grant Number:** 70NANB4H1073
Academic Institution: Carnegie Mellon University	**Major:** Physics (secondary: creative writing)
Academic Standing as of September '04: Sophomore	
Current Career Plans: Graduate school to continue physics studies	
NIST Laboratory, Division and Group: Physics Laboratory, Atomic Physics, Atomic Spectroscopy Group	
NIST Research Advisor: Dr. John Curry	
Title of Talk: Determining Plasma Temperatures with Spectroscopic Data	

Abstract of Talk:

Metal halide arc lamps are found in nearly 40 million lighting systems in North America alone. These energy-efficient, long-lived high intensity discharge lamps are used in warehouses, malls, and other commercial areas. Despite their popularity, detailed understanding of their operation is far from complete. Their color, intensity, and lifetime depend on the gas composition and plasma conditions inside the discharge tube. Spectroscopic observations can be used to probe these conditions, allowing for measurements of gas temperatures, densities, and species distributions. In this study, we use optical spectra acquired with a Fourier transform spectrometer to determine the plasma temperature at the core of a high-pressure mercury lamp doped with sodium iodide and dysprosium iodide. This lamp is one of a series of special test lamps constructed by Philips Research Laboratories, Aachen, Germany.

Prior to this project, an initial temperature had been determined using Karabourniotis's method, which examines the line profiles of self-reversed emission lines—that is, lines for which emitted photons are strongly absorbed before escaping the arc. Here, we use the relative intensities of optically-thin lines—those for which emitted photons escape the plasma without being reabsorbed—to determine temperature. If the plasma is in thermodynamic equilibrium, the relative population of atomic energy levels is a Boltzmann distribution at the equilibrium temperature. Therefore, the relative intensities of optically-thin lines contain information about the equilibrium temperature. By eliminating unsuitable lines (e.g., lines excessively widened by self-absorption, asymmetric lines, and lines whose classifications are considered uncertain), we arrive at a set of lines that produce linear Boltzmann plots. The resulting temperatures are lower than those determined from self-reversed lines; however, the emission intensities used in the analysis are line-of-sight measurements integrated across the entire lamp, so the data from the "center" of the lamp includes emissions far from the radial center. Since temperatures are lower farther from the arc core, this explains the low temperatures represented by the Boltzmann plots. To determine the intensities at the true core, we Abel-invert the data to produce a radial emission profile. This new intensity data is then plotted as before and results in temperatures somewhat higher than those determined by the self-reversed lines. Comparison of results from analyses of self-reversed lines and those obtained from analyses of optically thin lines provides information about the accuracy of various approaches and about deviations from local thermodynamic equilibrium inside the lamp.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Matthew A. Armstrong	**Grant Number:** 70NANB4H1056
Academic Institution: Davidson College	**Major:** Chemistry

Academic Standing as of September '04: Senior

Current Career Plans: Plan to go to graduate school, pursue studies in organic chemistry, and enter the pharmaceutical industry.

NIST Laboratory, Division and Group: Chemical Science and Technology Laboratory, Biotechnology Division, Bioprocess Measurements Group

NIST Research Advisor: Dr. Adolfas K. Gaigalas

Title of Talk: The Effect of Temperature on the Fluorescence of Phycoerythrin and Oligonucleotide-Labeled Fluorophores

Abstract of Talk:

A deeper understanding of the relation between conformations of biomolecules and the resulting fluorescence will provide scientists with useful tools for developing fluorescence labels and intensity standards. In the present study, we measured the temperature dependence of the fluorescence emission from fluorescein isothiocyanate (FITC) and rhodamine, both in solution and labeled with single and double-stranded oligonucleotides, and the temperature dependence of R-phycoerythrin (R-PE) and B-phycoerythrin (B-PE) fluorescence emissions. The fluorescence intensity changes were converted to quantum yield changes and analyzed in terms of phenomenological models. The two proteins contain numerous individual fluorophores in close proximity. Many of these fluorophores are attached to the protein backbone and have strong mutual interactions, which lead to significant changes in the fluorescence emission with changes in protein conformation. The small biomolecules, whose fluorescence behaviors are well established, exhibit similar interactions as the phycoerythrin when they are bound to varied strands of oligonucleotides. DNA-labeled FITC displays a temperature dependent fluorescence that is notably different from that of unbound FITC. Progress towards understanding of the relationship between protein conformations and their florescence will be presented.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Dahlia Ashford	**Grant Number:** 70NANB4H1040
Academic Institution: Mississippi State University	**Major:** Biological Science
Academic Standing as of September '04: Junior	
Current Career Plans: Plan to go to graduate or medical school to pursue studies in microbiology.	
NIST Laboratory, Division and Group: Building and Fire Research Laboratory, Materials and Construction Research Division, Inorganic Materials Group	
NIST Research Advisor: Dr. Jeff Bullard	
Title of Talk: The Influence of Chemical and Environmental Factors on Measurements of the Degree of Hydration of Cement Pastes	

Abstract of Talk:

The amount of reaction of cement with water, which is called the degree of hydration (DOH), influences the engineering properties of mortar and concrete. The DOH is commonly measured macroscopically by using one of several indirect methods such as non-evaporable water content, adiabatic heat signature, and chemical shrinkage. One disadvantage of such indirect methods is the uncertainty in how the conditions of the measurement affect the result. Variations in environmental factors such as temperature, carbon dioxide, and relative humidity all can influence the measurement of DOH. In this project, the non-evaporable water was measured for two cements as a function of time, curing temperature, and mixing proportions. The cements were cured at either 23 ºC or 60 ºC, and the influences of carbon dioxide and humidity on non-evaporable water were determined.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: William Ashley	**Grant Number:** 70NANB4H1064
Academic Institution: University of San Diego	**Major:** Computer Science

Academic Standing as of September '04: Junior

Current Career Plans: Plan to attend graduate school for an M.S. in software engineering.

NIST Laboratory, Division and Group: Information Technology Laboratory, Computer Rorensics Tools Testing Project

NIST Research Advisor: Steve Mead

Title of Talk: Verifying Deleted File Recovery Tools

Abstract of Talk:

Deleted file recovery tools provide computer forensics investigators with a time-saving means for increasing the amount of evidence they can present with their case. However, due to the complexity of recovering deleted files, it is not clear how well, or accurately these tools work.

The Computer Forensic Tool Testing project at NIST is a neutral third-party that develops specifications and testing methodologies for a variety of computer forensic tools -- including deleted file recovery tools. My area of research centered around contributing to a software framework being developed to measure and assess how well deleted file recovery tools function. Our methodology, progress and interesting preliminary results will be covered.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Whitney B. Austin	**Grant Number:** 70NANB4H1057
Academic Institution: Jackson State University	**Major:** Computer Science
Academic Standing as of September '04: Senior	
Current Career Plans: Plan to pursue graduate studies in computer science with a concentration in computer graphics and visualization.	
NIST Laboratory, Division and Group: Information Technology Laboratory, Mathematical and Computational Sciences Division, Scientific Applications and Visualization Group	
NIST Research Advisor: Mr. Steven G. Satterfield	
Title of Talk: Tracker Calibration for Immersive Visualization in a Reconfigurable Automatic Virtual Environment	

Abstract of Talk:

The use of immersive visualization is increasing rapidly within the scientific community. This is largely attributed to its widespread multi-disciplinary applications. To achieve a believable immersive experience, the users' position within the environment must be precisely known. This is accomplished through tracking systems. Unfortunately, these trackers are not always accurate. This paper describes a technique for calibrating electromagnetic tracking systems for immersive environments. The technique involves collecting sample points reported from the tracker and later comparing it with physical points. By mounting a sensor atop a crate apparatus, the physical and reported positions can be compared and analyzed. An evaluation of the technique looks to determine if this method of calibration is effective in improving the immersive experience of a user. Improving the accuracy of electromagnetic trackers allows for a better immersive visualization, and enables, scientific discovery to be achieve more quickly and efficiently.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Han Yong Ban	**Grant Number:** 70NANB4H101044
Academic Institution: Pomona College	**Major:** Physics
Academic Standing as of September '04: 1st year graduate student	
Current Career Plans: Finish graduate school and eventually work in government, industry, or academia.	
NIST Laboratory, Division and Group: Physics Laboratory, Electron and Optical Division, Electron Physics Group	
NIST Research Advisor: Dr. Jabez J. McClelland	
Title of Talk: Lifetime Measurement of Erbium Transition $4f^{12}6s^2 \rightarrow 4f^{11}(^4I^o_{15/2})\,5d_{5/2}\,6s^2$	

Abstract of Talk:

In the search for faster and faster processing speeds, the industry has been working to produce smaller and smaller semiconducting materials. In the near future, the industry will be mass producing semiconducting materials in the nanoscale. Currently used doping methods—which randomly distributes dopant atoms—will become insufficient for the production of materials in the nanoscale due to the variation in the number of dopant atoms present. A single atom doping method would have to be developed to produce semiconducting materials of this scale. The first step towards single atom doping would involve isolating and trapping a single atom. A few years ago, the Electron Physics group at NIST successfully trapped chromium atoms using a MOT (Magneto-Optical Trap). Similar trapping techniques can be used to produce single atoms of other elements.

This summer, I am working on the initial stages of a setup that would cool and trap single erbium atoms. For our experiment, it is important to know the lifetime of the particular transition that we are going to use to cool and trap the atom (in our case $^3H_6 \rightarrow \{15/2, 3/2\}^o$, at 841 nm). While lifetime measurements have been made for many atomic species, no measurement of our desired transition exists in the literature. We have constructed a vacuum chamber containing an Er evaporator, which is our atomic beam source. Light from a Ti:sapphire laser is used to excite the atom beam and the decay of the resulting fluorescence is measured to yield the lifetime. Progress and results will be discussed.

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NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Caitlin E. Baum	**Grant Number:** 70NANB4H1043
Academic Institution: University of Maryland, Baltimore County	**Major:** Biochemistry

Academic Standing as of September '04: Sophomore

Current Career Plans: I plan to go to graduate school to receive a degree in the field of Chemistry or Biochemistry.

NIST Laboratory, Division and Group: Building and Fire Research Laboratory, Fire Research Division, Materials and Products Group

NIST Research Advisor: Dr. Rick Davis

Title of Talk: Characterizing Polymer Nanocomposites During Processing

Abstract of Talk:

There is a demand in industry for polymers that are more fire resistant while still maintaining their mechanical and physical properties. Since most flame retardants are used in very high concentrations, many of the properties of the final product are significantly degraded. Dispersed organically modified layered silicates (organoclays) are unique in that they improve both the fire resistant properties and the mechanical properties of the polymer when incorporated into the polymer in relatively low concentrations. The end-product properties depend on the degree of organoclay dispersion and concentration, which currently can only be determined by time-consuming post-characterization (transmission electron microscopy, thermalgravimetric analysis, powder x-ray diffraction). We are working on an analysis technique that could be incorporated in a real-time, in-line process to analyze the final product while it is being extruded. The nanocomposites are primarily analyzed in terms of their visible color and fluorescent properties. This procedure would allow the operator in an industrial setting to adjust the processing conditions as needed to ensure an optimal product. By being able to immediately analyze the characteristics of the nanocomposite, companies can greatly reduce the waste of materials and time that was previously associated with post-extrusion analysis.

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NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Ben Baumgold	**Grant Number:** 70NANB4H1008
Academic Institution: Massachusetts Institute of Technology	**Major:** Materials Science Engineering Mechanical Engineering
Academic Standing as of September '04: Sophomore	
Current Career Plans: Explore various academic areas of interest to determine the focus of my studies.	
NIST Laboratory, Division and Group: Materials Science Engineering Laboratory, Metallurgy Division	
NIST Research Advisor: Dr. Robert Shull	
Title of Talk: Magnetic Refrigeration: Perfecting the Process	

Abstract of Talk:

Currently, conventional refrigeration technology cyclically pressurizes and depressurizes Chlorofluorocarbons (commonly known as Freon) to provide cooling in modern air conditioners and kitchen refrigerators. One of the main problems with this process is the unavoidable leakage of Freon into the atmosphere, causing ozone depletion and pollution. Additionally, current refrigeration cannot easily reach temperatures below 30 K (-405° F), which are necessary for satellite sensor cooling and hydrogen liquification (for the future fleet of hydrogen-powered cars) without multi-stage cooling that can be grossly inefficient.

An exciting and revolutionary alternative to the presently inefficient and environmentally harmful conventional refrigeration is magnetic refrigeration. This technology is based on the magnetocaloric effect of a material (the temperature change of that material due to the alignment of its magnetic spins when subjected to a magnetic field). Prototype magnetic refrigerators use metal alloys and permanent magnets to exploit this effect. A metal alloy is cyclically magnetized and demagnetized to provide powerful and efficient cooling without damage to the earth's atmosphere. The alloy is placed in the cooling chamber and a strong magnetic field is applied to magnetize the substance, thereby increasing its temperature but cooling the surrounding air in the refrigeration compartment. Then the material is removed from both the cooling chamber and the magnetic field. This allows the atomic spins to return to a disordered state and the stored heat to be released, preparing the material for another cycle of cooling. Magnetic refrigeration is both nondestructive and theoretically more efficient than either vapor expansion or radiant cooling.

In order to optimize the cooling effects of a magnetic refrigerator, a metal alloy must be found that exhibits optimal magnetocaloric effects at temperature ranges of interest. A recent publication in *Nature* ("Hysteresis losses in $Gd_5Ge_2Si_2$ by addition of iron", *Nature*, Volume 429, 24 June 2004, pages 853-857) shows that certain compounds, doped with iron, possess greatly enhanced effects. This project was focused on examining Holmium-Titanium-Germanium (HoTiGe) alloys doped with iron under the prediction they would also possess similar enhancements. Improved cooling potential around 90 K (-298° F) was previously documented by a group of Dutch scientists ("Magnetic-phase transitions and magnetocaloric effects", *Physica B*, Volume 319, 15 February 2002, pages 174-192). This summer, we revisited the Dutch research and found large magnetocaloric effects on this particular system at 15 K (-433° F) and 2 K (-456° F) as well. Further, we have identified the specific phase of the alloy that is responsible for these low-temperature magnetocaloric effects, $Ho_{58}Ti_5Ge_{36}Fe$. These results could have a major impact on low-temperature cooling techniques in the future by greatly improving the efficiency of magnetic cooling at low temperatures.

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August 10 – 12, 2004

Name: Daniel S. Blanchard	**Grant Number:** 70NANB4H1065
Academic Institution: Millersville University	**Major:** Computer Science
Academic Standing as of September '04: Senior	
Current Career Plans: Plan to go to graduate school to pursue Ph.D. in computer science.	
NIST Laboratory, Division and Group: Information Technology Laboratory, Information Access Division, Image Group	
NIST Research Advisor: Dr. Ross Micheals	
Title of Talk: Computer-Aided Camera Placement Software for Facial Recognition	

Abstract of Talk:

For computer vision systems requiring a rig of multiple cameras aimed at a target object, such as for redundant facial recognition, it is often useful to determine quantitatively what arrangement of cameras yields the most acceptable images over the largest area. Currently, there are no widely available programs that can be used to calculate this. This talk will describe a piece of software that utilizes a realistic camera model to aid in the design of camera rigs for facial recognition applications. The talk will outline the model in detail, propose results that verify its accuracy, present how the "operating envelope" is calculated, and conclude with a discussion of an optimal (application-specific) camera rig. The application may be easily customized for other multiple-camera applications.

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August 10 – 12, 2004

Name: Quenton Bonds	**Grant Number:** 70NANB4H1025
Academic Institution: Alabama State Universiy/University of Alabama at Birmingham	**Major:** Math/Electrical Engineering
Academic Standing as of September '04: Senior	
Current Career Plans: Plan to go to graduate school at USF to pursue studies in Electrical Engineering.	
NIST Laboratory, Division and Group: Electronics and Electrical Engineering Laboratory, Semiconductor Electronics Division, Electronic Materials Characterization	
NIST Research Advisor: Joeseph Kopanski	
Title of Talk: The Study of Metal Work Functions by Measurements of Capacitance-voltage, Scanning Kelvin Probe Microscopy	

Abstract of Talk:

This research focused on a brief and comprehensive study for determining different metal work functions by using capacitance-voltage (C-V), scanning Kelvin probe Microscopy (SKPM) measurements.

Three different metals such as chromium (Cr), silver (Ag), and aluminum (Al) were deposited on Si substrates by a thermal evaporator and then SiO2 layers were grown varying their thickness in the range of 5nm ~ 20nm. Through research of these methods, test structures and measurement capabilities can be developed to measure metal gate work functions with high accuracy.

The significance of these work function measurement methods apply to MOSFET Metal Oxide Semiconductor Field Effect Transistor technology. The accelerated growth of the semiconductor industry is based on the down-scaling of these MOSFET devices. Previously MOSFETs are based on the MOS/MIS (Metal Oxide/Insulator Silicon) structures with SiO_2 layer used as the oxide or insulator and polysilicon as the gate dielectric. By increasing the oxide capacitance these semiconductor devices can maintain functionality in microscopic forms. There are two ways to increase capacitance in these structures. The first would be to decrease the thinness of the oxide. The second method is to increase the dielectric constant. Currently oxide thicknesses have been theoretically scaled down to their smallest degree. Therefore extensive research is being conducted involving increasing the dielectric constant in such materials. This research uses what is called "High K Dielectrics", meaning the dielectric constant is drastically increased. In high k dielectrics, polysilicon is no longer used as the gate dielectric, metals are used. Therefore metal gate work function, compatibility with current MOS technology is a vital parameter for employing new gate electrode materials.

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NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Jennifer L. Breidenich	**Grant Number:** 70NANB4H1036
Academic Institution: Smith College	**Major:** Chemistry
Academic Standing as of September '04: Senior	
Current Career Plans: Work in the chemistry field for a year and then attend graduate school	
NIST Laboratory, Division and Group: Chemical Science and Technology Laboratory, Surface and Microanalysis Division	
NIST Research Advisor: Dr. Dave Holbrook	
Title of Talk: Investigating Interactions Between Colloidal Material and Polycyclic Aromatic Hydrocarbons: Quantifying Sorption Characteristics	

Abstract of Talk:

Polycyclic aromatic hydrocarbons (PAHs) are one of the most hazardous classes of hydrophobic organic contaminants, and are known to enter surface water through discharges from wastewater treatment plants. Toxins such as PAHs can be distributed throughout water in the particulate, colloidal, and dissolved phases. Colloidal material, usually defined as a solid material between 1 nm and 1 μm in size, has a large surface area that aids in its ability to bind to other colloids and dissolved species as well as PAHs. Interactions between colloids and PAHs are of interest because, although colloids make up only a small fraction of the total waterborne particle mass, their sorption to PAHs has the ability to enhance the transport, decrease the degradation rate, and reduce the bioavailability of the PAHs.

One of the main objectives of the experiment was to look for any temporal variation in the sorption coefficient in each of the samples. The second goal was to assess the impact of the wastewater discharge on colloidal material. Water samples from the Occuquan Watershed were taken before and after a wastewater treatment plant over a period of four weeks. A tangential flow filtration system separated the colloidal material from the dissolved material. A fluorescence quenching method was used to quantify the sorption coefficients of the colloidal matter for perylene, a model PAH.

A third goal of the research experiment was to determine if excitation-emission spectra could be used as a surrogate measure for quantifying colloidal sorption characteristics. Therefore, along with the fluorescence quenching data, the excitation-emission spectra for each of the samples was also collected and analyzed in order to look for any correlation between this data and the partition coefficient. Based on observations from the EES data and fluorescence quenching data combined, we hope that in the future colloidal investigations can use EES as a simple analytical tool in determining colloidal sorption characteristics.

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August 10 – 12, 2004

Name: Samuel M. Brewer	**Grant Number:** 70NANB4H1039
Academic Institution: Appalachian State University	**Major:** Physics with Astronomy concentration
Academic Standing as of September '04: Junior	
Current Career Plans: Plan to go to graduate school to pursue studies in physics.	
NIST Laboratory, Division and Group: Physics Laboratory, Atomic Physics Division, Plasma Radiation Group	
NIST Research Advisor: Dr. Endre Takacs	
Title of Talk: Visible Imaging of Highly Charged Ion Clouds in the NIST EBIT	

Abstract of Talk:

The NIST EBIT (Electron Beam Ion Trap) is an instrument for producing highly charged ions in a controlled environment and has long been used as a light source for spectroscopic measurements. The conditions of the ion cloud are similar to those found in the solar corona; however, the dynamics of the ion cloud itself are not fully understood. We have designed, setup, and used an imaging system using an intensified visible light CCD detector. Much can be learned about the spatial distribution, relative intensities, and possible cooling effects by imaging the ion cloud at various trap conditions. We will present preliminary results from this experiment.

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NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Charles Brooks	**Grant Number:** 70NANB4H1049
Academic Institution: University of Maryland	**Major:** Material Science and Engineering / Physics
Academic Standing as of September '04: Senior	
Current Career Plans: Graduate school in Material Science and Engineering	
NIST Laboratory, Division and Group: Material Science and Engineering Laboratory, Polymers Division, Electronics Materials Group	
NIST Research Advisor: Dr. Dean DeLongchamp	
Title of Talk: The Observance and Removal of PSS Top Layer in Poly(3,4-ethylenedioxythiophene)-polystyrenesulfonic Acid (PEDOT-PSS) Conducting Thin Films	

Abstract of Talk:

The polyelectrolyte complex, poly(3,4-ethylenedioxythiophene)-polystyrenesulfonic acid (PEDOT-PSS), is commonly used as a conducting polymer in organic electronic devices currently under intense research. The presence of a top layer in PEDOT-PSS films, deposited from an aqueous dispersion of PEDOT-PSS by spin-coating, has been observed. This was done by performing x-ray reflectivity and UV-VIS-NIR spectrophotometry before and after the removal of this top layer using an aqueous treatment. X-ray reflectivity provided sample thickness and roughness while UV-VIS-NIR spectrophotometry was used to obtain absorbance over a wide range of wavelengths. Film thickness after removal of the top layer decreases by between 30 to 40 % while optical absorbance decreases by only 5 to 11 percent. This indicates that the material in the top layer, the material being removed, is not responsible for the optical absorbance. Because the optical absorbance is primarily due to the conducting polymer PEDOT, the top layer is believed to be the electrically insulating polymer, PSS. The removal of this insulating top layer is critical to improving the charge transfer between interfaces involving PEDOT-PSS.

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August 10 – 12, 2004

Name: Shauntia Burley	**Grant Number:** 70NANB4H1067
Academic Institution: Coppin State University	**Major:** Mathematics and Computer Science
Academic Standing as of September '04: Senior	
Current Career Plans: Planning to pursue graduate studies in the field of Mathematics or Computer Science	
NIST Laboratory, Division and Group: Information Technology Laboratory, Mathematical and Computational Sciences Division	
NIST Research Advisor: Dr. Bonita Saunders	
Title of Talk: Creating 3D Visualizations for the NIST Digital Library of Mathematical Functions	

Abstract of Talk:

Several mathematicians and scientists at NIST have joined together with noted mathematical scientists throughout the U.S. and abroad on a tremendous project to establish a digital library of higher level mathematical functions. The Digital Library of Mathematical Functions (DLMF) is an ongoing project to update the extensive Handbook of Mathematical Functions which was originally published in 1964, edited by M. Abramowitz and IA Stegun, and issued by the National Bureau of Standards. This handbook is equipped with formulas, graphs, and mathematical tables for several mathematical functions which are also called "special functions".

The digital library will be taking a more in depth look at these "special functions" by allowing the user to interactively examine the unique features of these complicated mathematical functions through 2D and 3D visualization. Sometimes, the complex nature of these functions makes the task of visualization difficult. Many contain singularities and poles, which make the computational domains irregular, discontinuous, or multi-connected. This presentation will show how the use of contour plotting and grid generation techniques helps to facilitate the plotting of these complicated functions. This will allow the user of the digital library to gain a better understanding of how to use these high level functions to solve future problems in the mathematical and physical sciences.

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NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Alina Butler	**Grant Number:** 70NANB4H1040
Academic Institution: Mississippi State University	**Major:** Biology Pre-Med

Academic Standing as of September '04: Senior

Current Career Plans: Attend medical school and become a caring and successful emergency healthcare physician.

NIST Laboratory, Division and Group: Physics Laboratory, Ionizing Radiation Division, Radioactivity Group

NIST Research Advisor: Dr. Iisa Outola, Dr. Kenneth G. W. Inn, Hiromu Kurosaki, Svetlana Nour

Title of Talk: Evaluation of Alpha Spectra Deconvolution: A Beam Piercing Through the Vail of Obscurity

Abstract of Talk:

Working to uphold NIST's mission of advancing the United States' economic development, the Physics Laboratory works alongside industry to provide meaningful research for radiation usage. The radioactivity group supports innovative application of radiation through development of standard reference materials and measurement methods as one of several research programs. This program encompasses assessment of environmental and industrial emissions as a means of applying radiation control methods.

Alpha spectroscopy is the more commonly used method analyzing alpha energy, which is one of the more ordinarily found forms of radiation. A number of approaches have been used to evaluate alpha spectra. However, they all have flaws. The purpose of this experiment is to examine three different computer software and determine which of the three gives the more accurate result and which is easiest to learn, use, and is more time efficient.

In employing this experiment, nine samples of radionuclides were made using different isotopic ratios amounts (Americium 241/243, Thorium 229/230, Uranium 232/ Natural uranium). These ratios were one to one, one to three ratio, and one to ten ratio. To these samples were added varying amount of Neodymium carrier to give five, ten, and fifteen percent overlap between the resulting alpha peaks. The Americium and Thorium samples were co-precipitated directly then counted by alpha spectroscopy. On the other hand, the Uranium samples needed to be stripped of their daughter products using UTEVA Resin Columns, reduced using Titanium Tri-chloride, co-precipitated, and counted using alpha spectroscopy. Enough counts were collected to ensure a smooth spectra for analysis. After counting the samples, the resulting spectra peak areas were analyzed using Region of Interest, Genie-2000 Interactive Peak Fit, and WinAlpha (IAEA). The isotopic calculated and theoretical ratios were compared to give relative percent difference and percent uncertainty. Peak overlap was observed as well to study the effect of increased carrier amounts on accuracy and precision. Time efficiency, learning ability, and usage of the different software were taken into account to determine convenience of one software over the other.

Preliminary results seem to indicate that the both the Genie-2000 and WinAlpha software yield better accuracy and smaller uncertainty values than Region of Interest. However, both software require more time and effort for evaluation.

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August 10 – 12, 2004

Name: Mikolaj Bykowski	**Grant Number:** 70NANB4H1005
Academic Institution: Lehigh University	**Major:** Materials Science and Engineering
Academic Standing as of September '04: Senior	
Current Career Plans: Plan to go to graduate school to pursue studies in Materials Science and Engineering.	
NIST Laboratory, Division and Group: Materials Science and Engineering Laboratory, Metallurgy Division, Materials Performance Group	
NIST Research Advisor: Dr. William Luecke	
Title of Talk: Evaluating the Fire Resistance of Structural Steels	

Abstract of Talk:

This presentation will focus on the mechanical creep-ramp testing of standard and fire resistant construction steels and begin with the importance of being able to predict accurately the performance of steel in a real fire. A test similar to the mechanical tensile test was performed on various steel specimens, with the addition of a constant rate heating applied to the samples. This approach was intended to simulate the natural fire curve that occurs in building fires to better predict the behavior of specific structural members as opposed to the behavior of the entire structure. Various ramp rates were tested and comparison graphs were produced to observe trends in behavior. The failure criteria were characterized by a critical temperature, at which run-away strain occurred. The ultimate goal of this research is to be able to predict, based on the testing conditions, the fire resistance of steels. The microstructures of the samples before and after testing were also probed to discover any clues of predicting behavior under loading. An oxide layer formed in the tested samples due to the exposure to extreme heat. That oxide seemingly penetrated into the bulk of the sample along grain boundaries, which could indicate significant flaws in the material.

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August 10 – 12, 2004

Name: Daphne Chang	**Grant Number:** 70NANB4H1075
Academic Institution: Duke University	**Major:** Physics
Academic Standing as of September '04: Senior	
Current Career Plans: Graduate school in physics	
NIST Laboratory, Division and Group: Physics Laboratory, Ionizing Radiation Division, Radioactivity Group	
NIST Research Advisor: Hiromu Kurosaki	
Title of Talk: In Search of Higher PU Sensitivity for TIMS	

Abstract of Talk:

As an indicator of environmental health and national security, an accurate measurement of radionuclides in the environment is very important. One important goal in the analysis of radionuclide concentration is to maximize measurement sensitivity. To do so, many methods have been proposed and tried. This project aims at exploring the method of thermal ionization mass spectrometry (TIMS) for small sample analysis of plutonium. It is important in plutonium analysis to accurately measure isotopic ratios. The detection limit of TIMS for two different source loading techniques—direct loading, and electrodeposition— is investigated by varying the amount of plutonium source loaded into the machine. The TIMS detection limit for electroplating of plutonium onto filaments with a decreased surface area is also explored. This analysis provides a baseline for the current detection limit, which we aim to reduce by a couple orders of magnitude.

In addition, the resin bead loading technique for TIMS analysis is experimented. When executed correctly, this technique is purported to have the best sensitivity. So far, obstacles such as efficient loading of source onto the resin bead, transferring the bead onto the filament, and keeping the bead secured on the filament for the duration of the analysis, has rendered our attempts at resin bead loading unsuccessful. I will be exploring new ways to secure the bead onto the rhenium filament, and hope to present those results.

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August 10 – 12, 2004

Name: Andrew Q. Chereck	**Grant Number:** 70NANB4H1022
Academic Institution: Illinois Wesleyan Univ.	**Major:** Physics
Academic Standing as of September '04: Graduated	
Current Career Plans: Find a job in aerospace as an engineer or technician	
NIST Laboratory, Division and Group: Electronics and Electrical Engineering Laboratory, Quantum Electrical Metrology Division, E-Kilogram	
NIST Research Adviser: Dr. Richard Steiner	
Title of Talk: Controlling a Josephson Junction Array with LabView	

Abstract of Talk:

In the modern world it is becoming increasingly important to have accurate measuring devices. These devices derive their accuracy from the standards of length, time, mass, etc. Today, the only standard of measurement still based upon a physical artifact is the kilogram. A 1 kg (by definition) piece of platinum-iridium alloy sits in a vault in Paris, France. It has only been measured 3 times since its creation over 100 years ago. All of the prototype kilograms created at that time have been measured over the years and their mass has varied from the original, tending towards an average increase in mass by the prototypes. In an effort to lower the long-term error of the mass standard, a new approach is being worked out based on quantum sources and the relation of Planck's constant, h, and the speed of light, c. Since $E=m*c^2$ where m is mass and also $E=h*f$ where f is frequency, then m can be solved for giving $m=h*f/c^2$.

An important reference, the voltage source must be accurate and reproducible. In contrast to a battery, a Josephson effect voltage source is the most accurate voltage source known today thus lessening the overall error in determining the correct value for a mass of 1 kg. In order to effectively control the voltage source known as a Josephson Junction Array and to increase the efficiency and accuracy of data collection many different Labview routines must be written. Updating the original control program written in QuickBASIC involves interacting with 13 current sources for the JJ Array, a digital voltmeter, a current source, and a microwave power source.

Issues that need consideration are: finding the appropriate current operating point for each of 13 cells, verifying the voltage output, communicating with another control computer and effectively presenting the data in a user-friendly graphical interface.

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August 10 – 12, 2004

Name: Michelle N. Clarke	**Grant Number:** 70NANB4H1020
Academic Institution: Johns Hopkins University	**Major:** Mechanical Engineering
Academic Standing as of September '04: 1st year graduate student	
Current Career Plans: Completion of graduate studies in astronautical engineering	
NIST Laboratory, Division and Group: Building and Fire Research Laboratory, Materials and Construction Research Division, Inorganic Materials Group	
NIST Research Advisor: Dale Bentz	
Title of Talk: Characterization of the Microstructure and Properties of Fire Protective Materials	

Abstract of Talk:

The usefulness of specific fire protective materials (FPMs) cannot be quantified without a precise characterization of such properties as thermal conductivity, density, heat capacity, and other thermo-physical constants. To obtain these quantities, this project incorporated measurement techniques such as thermogravimetric analysis (TGA) as well as optical and scanning electron microscopy (SEM). X-ray microtomography captured 3d microstructure images. These were analyzed with finite element difference techniques to compute thermal conductivity. A clear relationship has been established between the microstructure and thermal performance of the FPMs used as building materials that protect steel. Data from the microstructure is used in a model developed to calculate thermal conductivities at various temperatures. This model and the information gathered will aid in the prediction of the performance of FPMs and affect the design of such materials in the industry.

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August 10 – 12, 2004

Name: Thomas E. Cleveland	**Grant Number:** 70NANB4H1041
Academic Institution: Tulane University	**Major:** Physics & Molecular Cell Biology double major
Academic Standing as of September '04: Sophomore	
Current Career Plans: Plan to go to graduate school for a Ph.D. in biophysics.	
NIST Laboratory, Division and Group: Physics Laboratory, Ionizing Radiation Division, Neutron Interactions and Dosimetry Group	
NIST Research Advisor: Dr. Muhammad Arif	
Title of Talk: Using Neutron Imaging to Analyze the Internal Structure of Biological and Mechanical Objects	

Abstract of Talk:

Much like x-rays, neutrons may be passed through an object to obtain a radiograph, revealing details of the object's internal structure. However, neutrons are absorbed by materials quite differently than x-rays. While x-rays are strongly absorbed by elements with high atomic number, neutron absorption is more complex and does not vary in a simple way with atomic number. Many light elements, of which hydrogen is the most important, absorb neutrons well enough to be imaged but are transparent to x-rays. Conversely, many common metals like aluminum and steel are more transparent to neutrons than x-rays. Because of these properties, it is often possible to obtain more detail from neutron radiographs than from x-ray radiographs. This is especially the case when it is necessary to image hydrogen-bearing compounds such as water and hydrocarbons; for example, imaging the transport of water in a hydrogen fuel cell.

While 2D neutron radiographs are useful in many circumstances, more information can be obtained by constructing 3D maps of an object's internal structure. If 2D radiographs of an object are taken at many different angles, computer algorithms can be used to reconstruct a 3D tomograph from all the 2D projections. Because of their ability to show many details of an object's internal structure, neutrons are especially suited to this process of computed tomography.

In this project, a portable and fully automated neutron tomography system was constructed. In the constructed system, the object to be imaged is placed on a computer controlled rotation stage, which rotates through the series of angles necessary for computed tomography. Thermal neutrons from the NIST reactor are passed through the object and impinge on a lithium-doped zinc sulfide scintillator screen, which is photographed by a computer controlled Apogee AP6 CCD. The system was used to image both mechanical and biological samples, including a hydrogen fuel cell and corn inoculated with *Aspergillus flavus*.

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August 10 – 12, 2004

Name: Daniel A. Cogut	**Grant Number:** 70NANB4H1054
Academic Institution: College of William and Mary	**Major:** Computer Science

Academic Standing as of September '04: Sophomore

Current Career Plans: Pursuing a double major in Computer Science and Mathematics

NIST Laboratory, Division and Group: Information Technology Laboratory, Statistical Engineering Division

NIST Research Advisor: Andrew Rukhin

Title of Talk: Fusion of Biometric Algorithms

Abstract of Talk:

Biometric identification plays an important role in security today. Biometric technology allows for recognition of an individual's identity based on certain characteristics, called signatures. These characteristics can include facial features, fingerprints, and vocal expressions. A signature of an unknown individual, called a probe, is compared to a database of known individual's signatures, called a gallery. Then a biometric algorithm produces similarity scores between the probe and each signature in the gallery and ranks them. Despite the fact that many biometric algorithms are now available for commercial use, there is no optimal algorithm that is widely accepted. Thus it is practical to create aggregations or fusions of various algorithms. In this project, the similarity scores produced by four biometric algorithms, with data from the Face Recognition Technology (FERET) program, were used. The method of fusion was implemented by means of weighted averaging of the ranks of the similarity scores.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 10 – 12, 2004

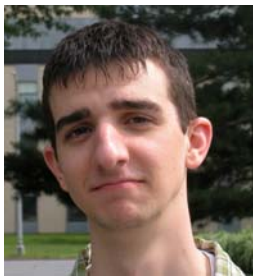
Name: April Colleton	**Grant Number:** 70NANB4H1035
Academic Institution: Rochester Institute of Technology	**Major:** Chemistry
Academic Standing as of September '04: Junior	
Current Career Plans: Plan to go to graduate school to pursue studies in organic chemistrry.	
NIST Laboratory, Division and Group: Chemical Science and Technology Laboratory, Process Measurement Division, Microfludic Group	
NIST Research Advisor: Dr. Rebecca Zangmeister	
Title of Talk: Electropolymerization and Functionalization of Polymeric Material for DNA Sensing in Microfluidic Channels	

Abstract of Talk:

Biologically friendly platforms are desirable for integration into microfluidic channels for sensitive and selective detection of biological species, such as DNA. In this project poly(3-aminophenol) was investigated as a possible substrate for DNA immobilization to be incorporated in a microfluidic channel system. 3-Aminophenol was electropolymerized at gold electrodes and investigated using reflection absorption infrared spectroscopy (RAIRS), contact angle, and X-ray photoelectron spectroscopy (XPS) measurements. The electrodeposited poly(3-aminophenol) layer was found to be insulating, and remains stable in aqueous solutions. It has been reported that 3-aminophenol electropolymerizes through the oxygen groups, allowing for subsequent chemical attachment of ssDNA probe molecules through the pendant amine groups.

Our strategy is to activate the amine groups of the poly(3-aminophenol) with glutaraldehyde that can further react with amine terminated ssDNA probe molecules, attaching them to the polymer surface. The ssDNA probe modified surface can then be used as a hybridization assay substrate to screen for fluorescently tagged ssDNA target molecules in an analyte solution. Electropolymerization of 3-aminophenol onto patterned electrodes will allow for spatial resolution of multiple probe-target. Integration of the patterned hybridization assay substrate surfaces within a microfluidic channel will make it possible to simultaneously run multiple DNA detection assays that will require minimum solution volumes.

Characterization of electropolymerized 3-aminophenol at gold electrodes, and subsequent immobilization of probe ssDNA for hybridization assays will be discussed.



SURF Student Colloquium

NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Jeffrey R. Comer	**Grant Number:** 70NANB4H1031
Academic Institution: University of Akron	**Major:** Physics
Academic Standing as of September '04: Senior	
Current Career Plans: Obtain a Ph.D. in the field of computational physics and work in academia.	
NIST Laboratory, Division and Group: Manufacturing Engineering Laboratory, Precision Engineering Division, Nanoscale Metrology Group	
NIST Research Advisor: Dr. John A. Dagata	
Title of Talk: Fractional Kinetics in Atomic Force Microscope Assisted Oxidation of Zirconium Nitride	

Abstract of Talk:

Atomic force microscope assisted lithography is a reliable method for the production of nanoscale surface structures and has been applied to the fabrication of nanometer-scale electronics and optical devices [1]. In addition, this patterning technique shows promise as a means to modify protein adsorption and control cell growth on the surfaces of medical implants [2]. In this talk, the author presents a study of the local oxidation kinetics of zirconium nitride that describes not only AFM lithography, but also serves as a model for fast parallel writing techniques [3].

The addition of various proportions of nitrogen to the sputtering plasma used to deposit the thin-films modifies their crystal structure and electrical properties, which are determined through X-ray diffraction and four-point probe measurements. By employing a fractional kinetics [4] model, the author investigates the effects of the altered material properties and a range of applied voltages on diffusion during oxide growth. The model predicts the existence of power of time dependent rate constants [5], where the exponent $(\gamma-1)$ is related to the defect density of the material. From experimental data, the author determines that γ increases from 1.0 to 2.2 for films deposited with nitrogen flow rates from 0.0 sccm to 10.0 sccm. While the local oxidation kinetics of systems such as silicon are highly subdiffusive, with γ ranging from 0.12 to 0.4, and the features developed are usually less than ten nanometers high [6], the zirconium nitride system displays controlled oxide growth to heights of several hundred nanometers.

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[2] C. Galli, M. Collaud Coen, R. Hauert, V.L. Katanaev, P. Gröning, and L. Schlapbach, *Colloids and Surf. B* **26**, 255–267 (2000).
[3] M. Cavallini, P. Mei, Fabio Biscarini, and R. García, *Appl. Phys. Lett.* **83**, 5286–5288 (2003).
[4] I.M. Sokolov, J. Klafter, and A. Blumen, *Phys. Today*, November 2002, 48–54.
[5] A. Plonka, *Prog. Reaction Kinetics* **16**, 157–333 (1991).
[6] J. A. Dagata, F. Perez-Murano, G. Abadal, K. Morimoto, T. Inoue, J. Itoh, and H. Yokoyama, *Appl. Phys. Lett.* **76**, 2710 (2000).

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NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Brad R. Conrad	**Grant Number:** 70NANB4H1035
Academic Institution: Rochester Institute of Technology	**Major:** Physics

Academic Standing as of September '04: RIT Alumni & UMD Graduate Student

Current Career Plans: Physics Graduate School at the University of Maryland, College Park and "…to do crazy things, what other people would consider crazy things. There's so much fun to be had."~ R. Feynman

NIST Laboratory, Division and Group: Material Science and Engineering Laboratory, Polymers Division, Characterization and Development Group

NIST Research Advisor: Dr. Chad Snyder

Title of Talk: Time Domain Dielectric Spectroscopy Analysis of the Amorphous Phase in Semicrystalline Polycarbonate

Abstract of Talk:

The amorphous state of Bisphenol-A Polycarbonate was examined by time-domain dielectric spectroscopy, as a function of crystallization time over a frequency range of $1x10^{-4}$ Hz to $1x10^{4}$ Hz. The dielectric measurements were conducted around the glass transition temperature of Bisphenol-A Polycarbonate. These dielectric studies were performed on a series of samples that were partially melted and recrystallized so as to investigate the influence of secondary crystallization on the α relaxation, thereby probing the effects of crystalline constraints on the cooperative dipole motions in the amorphous fraction. Analysis of the constrained behavior was performed via fitting to the Havriliak-Negami, Vogel-Fulcher-Hesse-Tammann, and Arrhenius equations. Insights and suggestions concerning the amorphous phase's crystallization dynamics will be briefly discussed.

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August 10 – 12, 2004

Name: Brian G. Cordes	**Grant Number:** 70NANB4H1051
Academic Institution: Worcester Polytechnic Institute	**Major:** Mathematical Sciences
Academic Standing as of September '04: Senior	
Current Career Plans: I am planning to pursue a PhD in Applied Mathematics	
NIST Laboratory, Division and Group: Information Technology Laboratory, Statistical Engineering Division	
NIST Research Advisor: Dr. Ivelisse Aviles	
Title of Talk: Developing a Graphical Tool to Determine the Estimation Capacity of an Experimental Design	

Abstract of Talk:

In scientific research, the quality of the design of an experiment has a great deal of impact on the quality of the experimental results. Experimental design is concerned with exactly this: finding the most efficient method for obtaining the most amount of information about a process. By using a certain class of experimental designs called assembled designs, Aviles (2001) has focused on determining optimal designs for robustness experiments. Assembled designs are very useful to study a process in which batches are produced and samples are made. In this case, the batch-to-batch (between-batch) variance and the (sample-to-sample (within-batch) variance are known as the variance components. The goal of robustness experiments is to find the settings of the factors so that the process mean is on target and the variance is minimized. Location effects are effects on the response mean and dispersion effects are effects on the response variance. The model used in these scenarios is a linear mixed-effects model with two variance components (between-batch variation and within-batch variation).

The concept of the Precision Plot has been developed to help the scientist determine the expected effectiveness of a design. This is accomplished by identifying how large the dispersion effects and variance components must be in order for the design to detect them. That is, if smaller effects must be detected, then the experimental budget must be increased (i.e., need a larger design) or the level of confidence in our results is decreased (for this design). Similarly, resources could be saved by running a smaller experiment, if it is detected that the estimation capacity of a design is greater than what is practically needed. The work done this summer includes both refining the Precision Plot method and improving the presentation of the outputted results. Precision Plots are calculated using normal theory and asymptotic approximations. Research done in the future will include establishing the adequacy of the approximation when sample sizes are much smaller.

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August 10 – 12, 2004

Name: Matthew Davidson	**Grant Number:** 70NANB4H1007
Academic Institution: Catholic University	**Major:** Chemical Physics
Academic Standing as of September '04: Senior	
Current Career Plans: Earn a doctoral degree in physics.	
NIST Laboratory, Division and Group: Physics, Laboratory, Atomic Physics Division, Quantum Processes Group	
NIST Research Advisor: Dr. Gavin K. Brennen	
Title of Talk: Quantum Cellular Automata Architecture in an Optical Lattice	

Abstract of Talk:

Two obstacles in neutral atom optical lattice quantum computing are the physical limitations of the current lattice technology and difficulty in manipulating individual atoms within the lattice. New ideas have been proposed which will allow scientists to overcome these two limitations. Among these are quantum cellular automata (QCA) and improved quantum error correction concepts. QCA are used to perform quantum computations as a circuit-based system would, with one important distinction, the use of rules rather than gates. With QCA, a rule is applied over a large system without the need for localized selective interactions, which are difficult with current technology. The application of these rules yields quantum states in which information is transmitted or distributed over the quantum bits (qubits) of the system. Quantum error correction techniques depend on the ability to distribute quantum information beyond a single qubit. By spreading information among multiple qubits in a system, the effects of localized noise may be minimized, reducing the probability of error.

Our efforts focus on implementing quantum error correction using QCA within the framework of the optical lattice of trapped rubidium atoms. By coding simulations of quantum systems being processed with QCA rules, we show that the basic states essential for error correction can be generated using QCA. Building on this result, we consider several qubit configurations that will support intermediate steps of quantum error correction. Since these steps involve localized measurements which alter the quantum information in the system, we demonstrate QCA methods of performing operations on assembled quantum information and later distributing it to prevent these measurements from altering elements of the system unintentionally. Having determined that the initial and final states for error correction are possible with QCA, we propose an architecture for implementing this quantum error correction within a two-dimensional optical lattice.

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August 10 – 12, 2004

Name: Dustin Diez	**Grant Number:** 70NANB4H1016
Academic Institution: Rhodes College	**Major:** Physics
Academic Standing as of September '04: Graduate	
Current Career Plans: Medical Physics PhD	
NIST Laboratory, Division and Group: Manufacturing Engineering Laboratory, Intelligent Systems Division	
NIST Research Advisor: Dr. Nicholas Dagalakis, Dr. Jason Gorman	
Title of Talk: Calibration of a Micro Force Sensor for the Characterization of Compliant Mechanism MEMS	

Abstract of Talk:

The development of compliant mechanism microelectromechanical systems (MEMS) has resulted in several useful systems such as micro-scale nanopositioners and manipulators. However, the fabrication processes used to manufacture these MEMS have manufacturing errors such as tapered cross sections and large feature size tolerances. The errors in the fabrication of MEMS devices may translate into variations in the stiffness of the compliant mechanism and the output force of micro-scale actuators. Therefore, it is desirable to mechanically probe the MEMS devices in the direction of intended motion so that stiffness and force measurements may be taken. Commercially available instruments for measuring these parameters are currently unavailable. This presentation presents the initial steps of the design and characterization of an instrument to perform these measurements. The focus will be on the calibration of a micro force sensor with force and displacement resolution on the order of 50 μN and 20 nm, respectively. The calibration procedures and resulting data for the sensor will be discussed. In addition, future plans for using this sensor as a mechanical probe for MEMS testing will be presented.

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August 10 – 12, 2004

Name: Brendan Farrar-Foley	**Grant Number:** 70NANB4H101058
Academic Institution: The George Washington University	**Major:** Computer Science
Academic Standing as of September '04: Senior	
Current Career Plans: Plan to obtain a masters degree focusing on computer security.	
NIST Laboratory, Division and Group: Information Technology Laboratory, Computer Security Division (893)	
NIST Research Advisor: Wayne Jansen	
Title of Talk: PDA Forensic Tools: Overview and Analysis	

Abstract of Talk:

Digital handheld assistants, such as Personal Digital Assistants (PDAs), are becoming more affordable and common in the workplace. Thy provide highly mobile data storage in addition to computational and networking capabilities for managing appointments and contact information, reviewing documents, communicating via electronic mail, and performing other tasks. Individuals can store and process personal and sensitive information independently of a desktop or notebook computer, and optionally synchronize the results at some later time. As digital technology evolves, the capabilities of these devices also continues to improve rapidly, taking advantage of new forms of removable media, faster processors that consume less power, touch screens with higher pixel resolution, greater connectivity with other mobile devices (via Bluetooth and 802.11), and other components designed specifically for mobile devices.

When handheld device are involved in a crime or other incident, forensic specialists require tools that allow the proper retrieval and speedy examination of information present on the device. PDA forensics differs in several important ways from traditional computer forensics. For example, PDAs are designed for mobility, hence compact in size and battery powered; they store user data in volatile memory instead of a hard disk.
This report gives an overview of current forensic software designed for acquisition, analysis, reporting of data discovered on PDAs, and an understanding of their capabilities and limitations.

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August 10 – 12, 2004

Name: Nathan T. Fisher	**Grant Number:** 70NANB4H1049
Academic Institution: University of Maryland	**Major:** Mechanical Engineering
Academic Standing as of September '04: Junior	
Current Career Plans: Plan to go to graduate school to study mechanical engineering and advanced energy systems.	
NIST Laboratory, Division and Group: Materials Science and Engineering Laboratory, Polymers Division, Electronics Materials Group	
NIST Research Advisor: Dr. Dean DeLongchamp	
Title of Talk: Correlating HMDS (hexamethyldisilazane) Modified Silica Substrate Surface Characteristics to Thin Film Morphology of Poly(3-hexylthiophene)	

Abstract of Talk:

Poly(3-hexylthiophene), also P3HT, a promising organic semiconductor, is known to have a self-ordering, semi-crystalline structure, which results in high field-effect mobilities in thin film transistor applications. A correlation between the surface characteristics of the substrate and thin film morphology was explored. Oxidized silicon wafers were chemically grafted with 1,1,1,3,3,3-Hexamethyldisilazane to provide substrates with a wide range of hydrophobicity quantified by contact angle analysis with DI water. Controlling the kinetics of the grafting process proved difficult because of short reaction times. To control the hydrophobicity of the substrate, a near fully grafted surface (hydrophobic) was exposed to UV-generated ozone to destroy the hydrophobic methyl groups. The exposure time to ozone and the water contact angle of the substrate followed a linear trend. Chloroform and Chlorobenzene were used as solvents for regioregular P3HT. The polymer was deposited on the surface energy-controlled substrates by spin-coating. Atomic Force Microscopy, confirmed by X-ray reflectivity, was used to measure the surface roughness of the thin films, which proved to be quite constant and independent of the degree of hydrophobicity of the substrate. Both solvents were unable to wet extremely hydrophobic substrates. Annealing was used to study direct interactions between the surface of the substrate and the polymer. The surface energy-controlled surfaces were employed in follow-up experiments utilizing the alternative deposition techniques of dip-coating and drop-casting, which are expected to be more greatly surface energy directed than spin-coating.

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NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Amanda Frederick	**Grant Number:** 70NANB4H1029
Academic Institution: Miami University	**Major:** Mechanical and Manufacturing Engineering
Academic Standing as of September '04: First year graduate school	
Current Career Plans: Pursue a masters degree in mechanical engineering at University of Pittsburgh	
NIST Laboratory, Division and Group: Manufacturing Engineering Laboratory, Manufacturing Metrology Division, Machine Tool Metrology Group	
NIST Research Advisor: Dr. Alkan Donmez	
Title of Talk: Use of a Laser Vibrometer for Measuring Spindle Error Motion	

Abstract of Talk:

Spindle error motion is an important consideration for judging the accuracy of a spindle's axis of rotation. Error in a rotating spindle axis can cause numerous defects in a machined surface, including errors in location and surface finish, and consequently is an important measurement for many industrial machining applications.

Currently, non-contact capacitance gauges have been established as the most reliable means for testing spindle error motion; however, bandwidth and size limitations make these sensors insufficient for measuring spindles of small machines, or spindles operating at high speeds. This work looks at the application of a laser vibrometer as a means of overcoming the limitations of capacitance gauges. The laser vibrometer in use is another non-contact type measurement system. It has the ability to output both velocity and displacement signals, and a Labview data acquisition program has been developed to acquire the data in the necessary format. Previously developed Matlab routines are being used to analyze the data and generate spindle axis of rotation error motion plots, as well as calculating the associated error motion parameters (synchronous and asynchronous error). Current tests were conducted on a 5-axis machining center spindle operating at 10,000 rpm in order to gauge the vibrometer's accuracy with that of the previously used capacitance gauges.

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August 10 – 12, 2004

Name: Alexander Fried	**Grant Number:** 70NANB4H1062
Academic Institution: University of Pennsylvania	**Major:** Physics
Academic Standing as of September '04: Sophomore	
Current Career Plans: Plan to go to graduate school to pursue studies in physics.	
NIST Laboratory, Division and Group: Physics Laboratory, Atomic Physics Division, Atomic Spectroscopy Group	
NIST Research Advisor: Dr. Gillian Nave	
Title of Talk: Digital Image Plate Diagnostics for Use in Ultraviolet Spectroscopy	

Abstract of Talk:

The Atomic Spectroscopy Group is investigating the use of digital image plates as an alternative to photographic film for recording spectral lines in the ultraviolet region below 3000 Å. Phosphor image plates are widely used for x-ray imaging, but are unexplored for the detection of vacuum ultraviolet light. They are available in large sizes of 20x40 cm, have good resolution, and are made of a flexible material that can conform to curved surfaces. Image plates offer great promise as a means to measure line intensities much more accurately than conventional films. This is of interest since such data are necessary to measure the transition probabilities of atoms in excited energy states.

This project is part of a continuing effort to develop experimental and analytical techniques with the image plate technology. Spectra of hollow-cathode discharges in He-Ne-Cu and Pt-Ne, and of Deuterium lamps were collected using the Normal Incidence Vacuum Ultraviolet Spectrograph. Using the plates, we were successfully able to measure the wavelengths of spectral lines for these elements. Experiments which calibrated the plates' response to intensity suggest that it is linear with exposure time, but that the magnitude of the response is sensitive to the wavelength.

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August 10 – 12, 2004

Name: Ángel G. Fuentes-Figueroa	**Grant Number:** 70NANB4H1046
Academic Institution: University of Puerto Rico-Mayagüez Campus	**Major:** BS in Theoretical Physics

Academic Standing as of September '04: Graduate Student

Current Career Plans: Finish a PhD in Astronomy at Arizona State University and maybe go to space.

NIST Laboratory, Division and Group: Physics Laboratory, Ionizing Radiation Division, Radioactivity Group

NIST Research Advisor: Dr. Leticia Pibida

Title of Talk: Testing Software Packages For Gamma-Ray Spectrometry Measurements Using Germanium Detectors

Abstract of Talk:

As a part of a large effort to improve the accuracy for the activity calibrations of gamma-ray emitting sources using High Purity Germanium (HPGe) detectors, the Radioactivity Group at the National Institute of Standards and Technology (NIST) is investigating the performance of several software packages used in data analysis. The American National Standard for Calibration and Use of Germanium Spectrometers for the Measurement of Gamma-ray Emission Rates of Radionuclides (ANSI N42.14-1999) was used to perform the tests required to investigate software packages' performance used for gamma-ray spectrometry data analysis. Following the procedures described in this standard, tests of four different software packages were performed. The software packages tested were FitzPeaks (© 1991-1999 Jim Fitzgerald), GENIE-2000(© 2004 Canberra Industries), Colegram (© 1994-1996 LPRI) and GammaVision (© 2002 Advanced Measurement Technology). These tests are described in section eight of the ANSI N42.14-1999 standard and include testing of automatic peak-finding algorithms, doublet-peak finding algorithms, fitting algorithms and the assessment of the magnitude of coincidence summing among others.

These tests were performed for two new p-type High Purity Germanium Detectors. The setup and calibration for these two new detectors were made following the ANSI N42.14-1999 standard and corrections for the pole/zero cancellation, dc level, live time and elapsed time, energy resolution and peak-to-comptom ratio were applied. Efficiency curves for these two new detectors were performed using gamma-ray sources with various characteristic energies. Efficiency curves for two existing detectors were updated and new geometries were added that allow us to calibrate the test sources develop by NIST for the Department of Homeland Security (DHS). Results for these tests are presented here. Also the efficiency curves for the detectors and comparisons of the data between the different detectors are presented in this report. Conclusions on the performance of the software packages for different measuring situations will be discussed.

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August 10 – 12, 2004

Name: Jingsi Gao	**Grant Number:** 70NANB4H1070
Academic Institution: Delaware State University	**Major:** Mathematics and Computer Science
Academic Standing as of September '04: Senior	
Current Career Plans: Plan to go to graduate school to pursue studies in Math and Computer Science	
NIST Laboratory, Division and Group: Information Technology Laboratory, Advanced Network Technologies Division, High Speed Networking Technologies Group	
NIST Research Advisor: Dr. Kotikalapudi Sriram and Dr. David Griffith	
Title of Talk: Wireless Enhancement For Storage Networking	

Abstract of Talk:

A storage area network (SAN) is a high-speed special-purpose network that interconnects data storage devices with associated data servers on behalf of a larger network of users. Storage devices are connected to a central SAN switch by optical fibers using either Fibre Channel or IP protocol (iSCSI). It is thus possible to connect all of a data center's storage to all of its servers and to all of its electronic information users. The disk arrays and tape silos that compose the SAN are typically housed in a rented facility and must be widely spaced to allow access for maintenance and upgrades. This can lead to considerable capital costs in terms of floor space and the amount of cabling required. Allowing storage disk controllers to connect to the SAN switch over wireless channels can reduce both costs by eliminating cabling and allowing the possibility of tighter equipment packing.

In our research we propose the creation of a wireless SAN and analyze its benefits. The proposed wireless SAN consists of a SAN switch that is connected to multiple wireless access points that communicate with the storage devices. This network would save space and reduce overall costs by not requiring wired connections. Wireless SANS would also provide more freedom in the placement of storage devices. However, because the number of wireless access points is less than the number of storage devices, it is possible for user data requests to be blocked if all access points are busy. An important design goal is therefore to minimize the probability that a network access request will be blocked.

To model the wireless SAN performance, we developed a theoretical model of the network characteristics using queuing theory. We next created a C++ simulation of a wireless SAN and compared the results that we obtained from the simulation with results obtained from the theoretical model in order to verify the accuracy of our analysis. The simulation was used to study how the number of available access points and various traffic loads affects the overall blocking probability and compare the wireless SAN's cost with the cost of traditional non-wireless SANs. It was found that wireless SANs would be much more cost effective. The results of the simulation can be used to provide design guidelines for building future wireless SAN. Also the work would be extended to analyze different kind of wireless technology like Ultra Wide Band 802.11, etc.

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August 10 – 12, 2004

Name: Chris S. Garber	**Grant Number:** 70NANB4H1019
Academic Institution: Austin Peay State University	**Major:** Physics

Academic Standing as of September '04: Senior

Current Career Plans: Electrical Engineering in graduate school or work in law enforcement/forensic science.

NIST Laboratory, Division and Group: Electronics and Electrical Engineering Laboratory, Office of Law Enforcement Standards

NIST Research Advisor: Susan Ballou

Title of Talk: Forensic Ballistics: Checking the Performance of Integrated Ballistics Systems with the Standard Bullet and Casing Project

Abstract of Talk:

Firearms leave unique marks on fired bullets and casings that are ejected from their chambers. When examined by a firearm examiner, these unique signatures can link firearms to criminal activity. The FBI and ATF originally developed independent image capture, image analysis, and database systems to capture and store these unique signatures. The FBI system was called DRUGFIRE and the ATF system was called IBIS (Integrated Ballistics Identification System). In 1998 the two agencies agreed to use just one system, IBIS, and created the National Integrated Ballistics Information Network (NIBIN). By the end of 2002, IBIS systems had been installed in 233 U.S. crime labs slated to be part of the NIBIN.

One key idea of sharing firearms data between crime labs is the establishment of measurement standards for traceability, unification, and quality control. Through funding provided by the National Institute of Justice, The National Institute of Standards and Technology (NIST) is developing a virtual and physical bullet signature standard (RM8240) and casing signature standard (RM8250) to be used by crime labs across the world to check the performance of their integrated ballistic systems.

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August 10 – 12, 2004

Name: Lloyd W. Gewuerz	**Grant Number:** 70NANB4H1048
Academic Institution: Binghamton University, SUNY	**Major:** Mechanical Engineering

Academic Standing as of September '04: Senior

Current Career Plans: Plan to go to graduate school for an MBA and then possibly a degree in either biomedical or mechanical engineering

NIST Laboratory, Division and Group: Building and Fire Research Laboratory, Fire Research Division, Materials and Products Group

NIST Research Advisor: Dr. Greg Linteris

Title of Talk: The Capabilities of FDS for Prediction of the Steady-State Burning of Small-Scale Materials

Abstract of Talk:

The NIST Fire Dynamics Simulator (FDS) is a widely used program for predicting hot gas and smoke movement through a burning building. Recently, its use has been extended to include the prediction of fire growth and spread. In order to assess the usefulness of FDS for this purpose, an analysis of the burning of small-scale samples under controlled conditions is necessary. We have chosen to model the burning of polymethyl methacrylate (PMMA) in both the horizontal and vertical orientations within the cone calorimeter and at various known radiant fluxes. Furthermore, the properties of the material and other calculation parameters were varied to determine the importance of each for simulation accuracy. The parameters varied were: activation energy, pre-exponential factor, ignition temperature, domain size, LES/DNS calculation method, presence of hood vent air flow, and grid spacing.

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August 10 – 12, 2004

Name: Stephanie E. Goldfarb	**Grant Number:** 70NANB4H1013
Academic Institution: Cornell University	**Major:** Mechanical Engineering
Academic Standing as of September '04: Sophomore	
Current Career Plans: Plan to go to graduate school to pursue studies in Theoretical and Applied Mechanics	
NIST Laboratory, Division and Group: Building and Fire Research Laboratory, Materials and Construction Research Division	
NIST Research Advisor: Dr. Emmett O'Brien	
Title of Talk: Factors Influencing the Determination of the Strain Energy Release Rate of an Adhesive Tape	

Abstract of Talk:

In the pressure sensitive adhesive tape (PSAT) industry there is a need for agreement upon a standard method to determine adhesive properties such as the strain energy release rate, *G*. The *G* value, in units of joules per meter squared (J/m^2), quantifies the energy required to break a unit surface area of the adhesive bond between the PSAT and a rigid substrate. A variety of adhesion tests, models, and equations have been developed to determine *G*. The calculated *G* value often varies with the geometry of the test.

The effects of shaft tip and substrate hole diameters on the strain energy release rate, *G*, measured by the shaft loaded blister test (SLBT) were studied. The adhesive system consisted of samples of Kapton pressure sensitive adhesive tape (PSAT) adhered to a glass surface. The *G* value of the system was calculated using four equations: (1) load-based, (2) hybrid, (3) displacement-based, and (4) combination. The values calculated from the displacement and hybrid equations exhibit a significant dependence on the ball bearing and hole sizes. Both equations rely heavily upon the measured extension, *w*, of the shaft and the attached ball bearing. As the equations account for only elastic deformations of the adhesive surface, plastic deformation at the point of contact between the shaft tip and the adhesive results in an overestimation of *w*. Use of the combination equation for *G*, as it places less emphasis on the value of *w*, provides for a reduced sensitivity to plastic deformations of the PSAT. The load-based equation, which avoids consideration of the shaft extension altogether, provides for an accurate and consistent set of *G* data, independent of the geometry of the test.

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August 10 – 12, 2004

Name: William J. Goodrum, Jr.	**Grant Number:** 70NANB4H1059
Academic Institution: University of Virginia	**Major:** Mechanical Engineering
Academic Standing as of September '04: Sophomore	
Current Career Plans: Study for a Master's in ME, followed by a career in Motorsports	
NIST Laboratory, Division and Group: Materials Science and Engineering Laboratory, Polymers Division, Combinatorial Methods Group	
NIST Research Advisor: Dr. Steven D. Hudson	
Title of Talk: Microfluidic Interfacial Tension Measurements: Getting the Most From Your Soaps	

Abstract of Talk:

With the market demand for better household chemicals pressuring companies like Dow Chemical or Proctor & Gamble, the race is on to find cheaper and more effective measurement techniques to determine chemical properties. Companies need the ability to minimize wasted and potentially expensive reagents, while still giving their scientists the chance to ask those "What ifs?" that are so crucial to development. That is why microfluidic methods have stepped to the fore. This presentation intends to outline current developments at NIST in the measurement of Interfacial Tension (IFT) with microfluidic devices, while focusing on the processes and shortcomings of the industry standard pendant drop test. Specifically, results and conclusions based on dynamic surface tension measurements of various surfactant solutions using a pendant drop tensiometer will be presented, explained, and qualified. Also, a consideration of possible microfluidic applications and of current consumer products (i.e. Mr. Clean AutoDry Car Wash) will demonstrate the need and market potential for rapid, compact, high-throughput microfluidic testing devices.

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August 10 – 12, 2004

Name: Cornelius Griggs	**Grant Number:** 70NANB4H1049
Academic Institution: University of Maryland	**Major:** Materials Science and Physics
Academic Standing as of September '04: Junior	
Current Career Plans: Plan to go to graduate school to pursue studies in Materials Science.	
NIST Laboratory, Division and Group: Materials Science and Engineering Laboratory	
NIST Research Advisor: Dr. Brian Lawn	
Title of Talk: Investigating Mechanical Properties of Thin Films via Nanoindentation	

Abstract of Talk:

Knowledge of the mechanical properties of thin films, particularly silicon-based films, is important for many important applications, including semi-conductors and MEMS. Little is known about the changes in mechanical properties as the size of the material sample is reduced, yet these properties are crucial for device reliability.

In our work, nanoindentation is used to investigate basic material properties of oxide and nitride thin films on silicon substrates. Modulus, hardness, residual stress, and strength are studied. Equations have been developed to deconvolute film properties from tests on film substrate bilayers. Crack lengths resulting from nanoindentation are measured using AFM and are then used to predict film residual stress.

The effects of temperature, deposition power, pressure, and deposition temperature are compared. Films fabricated at lower temperatures tend to have lower modulus and hardness due to a lower density, though power and vacuum are also important factors. This method can be used to find optimal processing conditions to produce optical mechanical properties, for instance films that are strong with low residual stress.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Theodore Robert Harris	**Grant Number:** 70NANB4H1037
Academic Institution: University of North Carolina at Charlotte	**Major:** Electrical Engineering
Academic Standing as of September '04: Senior	
Current Career Plans: Pursuing higher education in electrical engineering	
NIST Laboratory, Division and Group: Materials Science Engineering Laboratory, Ceramics Division, Electronic and Optoelectronic Materials Group	
NIST Research Advisor: Dr. Peter Schenck	
Title of Talk: Combinatorial Study of Nickel-Gold p-contacts for Blue InGaN Light Emitting Diodes Comparing Electron Beam and Pulsed Laser Deposition Techniques	

Abstract of Talk:

Low resistance (ohmic) transparent contacts for light emitting diodes (LEDs) are increasingly needed for the success of blue and UV LEDs and laser diodes. Thin films of Ni and Au were deposited using pulsed laser deposition (PLD) and e-beam deposition systems onto sapphire. The optical characteristics were then evaluated by transmission and reflection spectroscopy. Different film ratios of Ni/Au and rapid thermal annealing (RTA) temperatures were explored. Additionally, a combinatorial study on the ratio of the thicknesses of Ni and Au in p-type contacts on blue LED wafers will be discussed.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Stacey J. Hoebel	**Grant Number:** 70NANB4H1053
Academic Institution: Univ. WI, Madison	**Major:** Biomedical Engineering
Academic Standing as of September '04: Senior	
Current Career Plans: Plan to go to graduate school to pursue studies in biomedical engineering, specializing in biomechanics and/or biomaterials.	
NIST Laboratory, Division and Group: Chemical Science and Technology Laboratory, Analytical Chemistry Division, Microfluidics Group	
NIST Research Advisor: Dr. David Ross	
Title of Talk: Temperature Gradient Focusing	

Abstract of Talk:

Several analytic methods are commonly used to concentrate, separate, and identify various chemical analytes in solution. While popular separation methods such as Isoelectric Focusing (IEF) and Capillary Electrophoresis (CE) are quite effective, they also have limited applications due to specific analyte requirements (i.e. pH, charge, size, etc.), entail extensive preparation including the pre-concentration of the analyte, and are often difficult to implement.

Temperature Gradient Focusing (TGF), an exciting new separation and concentration technique developed at NIST, has the ability to detect very dilute solutions of a wide variety of analytes using a relatively simple procedure. Concentration and focusing of the ionic species are performed in a tiny capillary or microfluidic channel by balancing the electrokinetic velocity of the analyte ions against the bulk flow of solution. A temperature gradient is applied to the capillary, creating a corresponding gradient in the electrokinetic velocity. The counterbalancing bulk flow rate can then be varied in such a way that the bulk and electrokinetic velocities sum to zero at a unique point, at which the analyte is focused.

The TGF technique has been effectively demonstrated for several analytes, including fluorescent dyes, amino acids, DNA, proteins, particles, and chiral molecules. However, validation of the repeatability of the technique as well as the establishment of an optimal operating procedure for quantitative measurements were necessary. To obtain accurate and efficient results using TGF, a scanning technique was developed. By manipulating the bulk flow through the capillary, the analyte peaks were systematically moved through a small region of the capillary. A camera captured images of each of the peaks (up to five analytes in each sample), which could be used to analyze the intensity/concentration of the sample. Many experiments were performed using this scanning technique to determine how various factors such as the steepness of the temperature gradient, the type of buffer used, the voltage applied, and the initial concentration of the analyte influence TGF scans for the separation of amino acids.

By the end of the summer, an optimal operating procedure was established for amino acid separations with TGF. This TGF procedure was then demonstrated for quantitative measurements of aspartame (a combination of two amino acids) and some of its degradation products in diet soda.

Since TGF can be used with any charged analyte and requires very low initial concentration, it has countless other potential uses. Possible applications of TGF include the identification and analysis of protein in urine for medical diagnosis and the detection of biological weapons such as anthrax.

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NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Michael Huber	**Grant Number:** 70NANB4H1038
Academic Institution: American University	**Major:** Mathematics and Computer Science
Academic Standing as of September '04: Junior	
Current Career Plans: Unknown	
NIST Laboratory, Division and Group: Information Technology Laboratory, Mathematical and Computational Sciences Divisioin	
NIST Research Advisor: Bonita Saunders	
Title of Talk: Streamlining the Production of Viewpoints in VRML	

Abstract of Talk:

The Handbook of Mathematical Functions, a reference book initially published in 1964 by NIST and its predecessor the National Bureau of Standards, provides definitions, tables, charts and graphs for many high level functions in Mathematics. The success of the Handbook of Mathematical Functions has led to a project that will massively update its content and presentation, named the Digital Library of Mathematical Functions. Its goal is to provide reference material for high-level functions in an electronic form, and to offer it on the internet.

A major aspect of this project is to provide 3D graphs of high-level functions in a format that will allow viewers to thoroughly examine as many aspects of the function as possible. This has been achieved through the use of the Virtual Reality Modeling Language (VRML). VRML allows a viewer to rotate, zoom, pan and otherwise manipulate a 3-Dimensional figure, which is optimal for viewing high-level functions.

The 3-Dimensional figures are prepared through such programs as Mathematica and Maple, and are translated into VRML, fine-tuned, and then finalized. This finalization process involves the graph being verified for its accuracy and put into a presentable form where many different vantage points are examined and set for the final product. We will discuss the production of these VRML images, and the production of a tool designed to streamline the process of selecting these viewpoints.

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August 10 – 12, 2004

Name: Nicholas R. Hughes	**Grant Number:** 70NANB4H1014
Academic Institution: Southern Methodist University	**Major:** Mechanical Engineering/Math
Academic Standing as of September '04: Senior	
Current Career Plans: Plan to get a job after graduation.	
NIST Laboratory, Division and Group: Materials Science and Engineering Laboratory, Polymers Division, Processing Characterization Group	
NIST Research Advisor: Dr. Frederick R. Phelan Jr.	
Title of Talk: Chaotic Mixing in Microfluidic Devices	

Abstract of Talk:

Microfluidic flows are normally low Reynolds number (Re) due to the very small length scales at which these devices are fabricated. This makes turbulent flow virtually impossible to achieve and the mixing of fluids is generally slow and diffusion controlled. Mixing can be greatly enhanced in the laminar flow regime by subjecting the fluid to chaotic flow kinematics. In chaotic advection, material lines undergo complex patterns of stretching and folding. Mixing is greatly enhanced both by the tendency of fluid particles to become homogeneously dispersed, and by a decrease in the length scale for diffusion between unlike components.

In this work, mixing in microfluidic devices in which flow in the streamwise direction is perturbed by oscillatory transverse flow has been studied. Numerical simulation of the unsteady Navier-Stokes equations has been used to determine combinations of flow geometries and boundary conditions which lead to chaotic mixing regimes. The flows are shown to be chaotic by the computation of positive Lyapunov exponents and by visual inspection of particle scatter when material lines undergo stretching and folding. A number of cases that show promise for future experimental work will be shown.

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August 10 – 12, 2004

Name: Jesse W. Hwang	**Grant Number:** 70NANB4H1049
Academic Institution: University of Maryland, College Park	**Major:** Biological Resource Engineering, Pre-medicine
Academic Standing as of September '04: Sophmore	
Current Career Plans: Plan to earn a Bachelor's degree in Biomedical Engineering and go on to either medical or dental school.	
NIST Laboratory, Division and Group: Materials Science & Engineering Laboratory, Polymers Division, Biomaterials Group	
NIST Research Advisor: Dr. Ming Tung	
Title of Talk: Development of Calcium Phosphate-gelatin Composites	

Abstract of Talk:

This study was performed to investigate and develop a biomaterial of calcium phosphate/gelatin to be used as an injectable bone substitute. Gelatin is an ideal medium to transfer calcium phosphate because it is biocompatible, biodegradable, cheap, and can be injected without open surgery. The interaction of calcium and phosphate with gelatin will be studied; these include solubility, titration and precipitation. The calcium phosphate/gelatin composites will be characterized by chemical analysis, x-ray powder diffraction, and infrared spectroscopy. The mechanical strength, such as DTS, will also be investigated.

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NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Teresa L. Jacques	**Grant Number:** 70NANB4H1036
Academic Institution: Smith College	**Major:** Chemistry
Academic Standing as of September '04: Junior	
Current Career Plans: Graduate school to pursue studies in forensic chemistry or mineralogy	
NIST Laboratory, Division and Group: Materials Science & Engineering Laboratory, NIST Center for Neutron Research, Neutron Condensed Matter Science Group	
NIST Research Advisor: Dr. Sushil Satija	
Title of Talk: X-ray Reflectivity Study of the Formation of Alkane Films on OTS-coated Silicon Surfaces	

Abstract of Talk:

The study of thin films on the nanometer or Ångstrom scale has a great deal of applications in materials science. Within this field, there is much interest in the interactions between organic molecules and a variety of substrates, as the mechanisms of many of these interactions are not well understood. Silicon substrates are often used to study such interactions due to the ease with which their surfaces can be chemically modified to suit an experiment. In this experiment, silicon wafers were coated with a self-assembled monolayer (SAM) of octadecyltrichlorosilane (OTS). Heptane was used to wet the surface of this new substrate. The procedure for growing these layers will be briefly described.

X-ray and neutron reflectometry are powerful techniques that can elucidate the thickness and roughness of thin films. X-ray reflectometry is used in this experiment to probe these characteristics of the heptane film on the OTS layer. The behavior of such films is extremely sensitive to temperature stability, making temperature control of paramount importance in this experiment. It is critical that the temperature be stable across the substrate to ensure that the film is the uniform over the entire sample. The measures that were taken to ensure temperature stability of the sample within 1mK will be explained.

The wetting behavior of heptane on OTS as a function of temperature will be examined and the results compared to those of recent ellipsometry studies of alkane wetting behavior on silane-covered silicon substrates.

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August 10 – 12, 2004

Name: Firouzeh Jalilian	**Grant Number:** 70NANB4H1049
Academic Institution: University of Maryland, College Park	**Major:** Computer Science
Academic Standing as of September '04: Senior	
Current Career Plans: Plan to go to graduate school to pursue studies in Computer Science.	
NIST Laboratory, Division and Group: Information Technology Laboratory, Statistical Engineering Division	
NIST Research Advisor: Alan Heckert	
Title of Talk: Developing a Graphical User Interface for the Mass Calibration Program	

Abstract of Talk:

The Statistical Engineering Division and the Manufacturing and Metrology Division are rewriting the Masscomp program that is used to assign mass values to weights submitted to NIST for calibration. The current production software was written in 1970s using the programming language Fortran 66. The code is being modernized to Fortran 90. However, the program could only be run in a shell such as MS DOS. My project has been to develop a Graphical User Interface for this calibration program in order to make it easier to use. Different approaches were investigated and it was decided that the programming language Visual Basic would be most suitable for developing this interface. In addition to learning Visual Basic (VB) and Fortran 90, I also had to learn Fortran/Visual Basic Mixed-Language programming. The project involved creating a Fortran Dynamically Linked Library (DLL) and exporting its routines into VB. These routines could be called by VB during execution of the graphical user interface. The next stage of the project is to add a feature that plots the results at the end of the program. Once completed, this graphical user interface will make it significantly easier and faster to use the Masscomp program. In addition, Visual Basic proved to be versatile tool for developing a graphical user interface.

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August 10 – 12, 2004

Name: Dyami H. Jenkins	**Grant Number:** 70NANB4H1049
Academic Institution: University of Maryland – College Park	**Major:** Computer Science
Academic Standing as of September '04: Senior	
Current Career Plans: Plan to go into industry for a few years before attending graduate school to pursue studies in finance and marketing or information technology consulting.	
NIST Laboratory, Division and Group: Information Technology Laboratory, Computer Security Division	
NIST Research Advisor: Lawrence E. Bassham	
Title of Talk: Augmentation of the Statistical Test Suite for Random Number Generators	

Abstract of Talk:

This talk focuses on changes that were made to statistical test suite and the testing that was conducted using the modified version. In addition, the talk discusses some aspects of selecting and testing random and pseudorandom number generators. The outputs of such generators may be used in many cryptographic applications, such as the generation of key material. Generators suitable for use in cryptographic application may need to meet stronger requirements that for other applications. In particular, their outputs must be unpredictable in the absence of knowledge of the inputs. Some criteria for characterizing and selecting appropriate generators are discussed. The subject of statistical testing and its relation to cryptanalysis is also discussed, and some recommended statistical tests are provided. These tests may be useful as a first step in determining whether or not a generator is suitable for a particular cryptographic application. However, no set of statistical tests can absolutely certify a generator as appropriate for usage in a particular application, i.e., statistical testing cannot serve as a substitute for cryptanalysis.

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August 10 – 12, 2004

Name: Soren Johnson	**Grant Number:** 70NANB4H1061
Academic Institution: Boston University	**Major: Computer Science**
Academic Standing as of September '04: Senior	
Current Career Plans: Undecided.	
NIST Laboratory, Division and Group: Information Technology Laboratory, Computer Security Division	
NIST Research Advisor: Tom Karygiannis	
Title of Talk: An Intrusion Detection System in a Wireless Ad Hoc Network	

Abstract of Talk:

Our group considered an intrusion detection system in a wireless ad hoc network. Such a network does not have any hardware dedicated to routing packets, so each node must participate in routing and passing other nodes' packets along. Because such a network relies on cooperation between nodes, routing security is difficult to ensure. If a node is compromised, it could start dropping data packets instead of forwarding them to create a disruption. Also, a node could change data packets to compromise data integrity.

Our project consisted of developing an intrusion detection system whereby each node observes and reports on misbehavior in neighboring nodes. Each node observes the packets coming into and out of its neighbors and making sure that each one was forwarded properly. If more than a certain threshold of packets are dropped or mangled, the observing node must report this to the rest of the network. This would allow a higher level protocol to respond by routing data packets around offending nodes and blocking their participation in the network. My specific portion dealt with the reporting of malicious behavior via "accusations". Once a node detects a malicious neighbor, it broadcasts a digitally signed message reporting the event. However, we must beware that compromised nodes cannot cause a node to be excluded from the network using false accusations. Therefore, when a node receives an accusation, it must check to see whether it can see the accused node and, if so, whether that node is, in fact, committing malicious acts. If a node finds that one of its neighbors is falsely accused, it must accuse the accuser of false accusation. In this way, even if a node or a few nodes are malicious, they will be detected by their neighbors and reported to the network.

Some further work involved distinguishing the malicious dropping of packets from packet drops due simply to a poor connection. I developed a tool to detect signal strength between wireless nodes, which can later be used to dynamically adjust the threshold so that poorly connected nodes aren't considered malicious.

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August 10 – 12, 2004

Name: Eric D. Kelsic	**Grant Number:** 70NANB4H1074
Academic Institution: California Institute of Technology	**Major:** Physics
Academic Standing as of September '04: Junior	
Current Career Plans: no idea. grad school?	
NIST Laboratory, Division and Group: Physics Laboratory, Electronic and Optical Physics Division	
NIST Research Advisor: Dr. Charles W. Clark	
Title of Talk: Efficient Implementation of Error-Handling for Quantum Key Distribution	

Abstract of Talk:

Quantum cryptography systems are perfectly secure in theory, but their practical implementation produces key errors at a level unacceptable for data encryption. Thus the reconciliation of the sender's (Alice's) and receiver's (Bob's) key becomes an essential element of the cryptographic system. Previous implementations (CASCADE) have emphasized high percentage bit preservation at the cost of processing power. NIST's quantum key distribution system uses faster error-correcting Hamming codes to correct 1-bit errors and detect multiple bit errors, decreasing the percentage of retained bits but speeding up the overall rate of error correction. My project is to implement the error-correction algorithm in the C language (inherently faster than previous implementations in Java), allow multiple processes to run concurrently (which decreases the wait time for between Alice-Bob communications), and provide a framework for eventual optimization of the algorithm. The final program will be used in the second generation key distribution system, which is attempting to achieve the major milestone of encrypted streaming video transmission.

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August 10 – 12, 2004

Name: Meeri N. Kim	**Grant Number:** 70NANB4H1061
Academic Institution: Boston University	**Major:** Physics
Academic Standing as of September '04: Graduated	
Current Career Plans: Plan to go to graduate school to pursue studies in physics.	
NIST Laboratory, Division and Group: Physics Laboratory, Atomic Physics Division, Laser Cooling and Trapping Group	
NIST Research Advisor: Dr. Paul Lett	
Title of Talk: Searching for Evidence of Correlated Photons Formed by 4-Wave Mixing	

Abstract of Talk:

Correlated photons can be applied in such areas as quantum mechanical testing and quantum cryptography. For two photons to be correlated, they must be theoretically produced at the exact same moment in time. One method of production is degenerate 4-wave mixing. Two intense beams of laser light—called pump beams—along with a weaker probe beam intersect in a heated glass cell filled with rubidium atoms. As a result of a 4-wave mixing process involving induced gratings and diffraction, a "cone" is emitted from the cell that consists of opposing pairs of correlated photons, and a beam conjugate to the probe appears. Unlike the correlated photons formed by parametric down conversion, these pairs have the same frequency that can be tuned accordingly. The current challenge is to find evidence of this correlation via photon counting methods, and then to utilize a Bose-Einstein Condensate to create beams of correlated atoms.

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August 10 – 12, 2004

Name: Carolyn A. Kitchens	**Grant Number:** 70NANB4H1039
Academic Institution: Appalachian State University	**Major:** Chemistry Pre-professional
Academic Standing as of September '04: Senior	
Current Career Plans: Plan to attend graduate school and pursue a Ph. D/MD in Biomedical Engineering.	
NIST Laboratory, Division and Group: Chemical Sciences and Technology Laboratory; Surface and Microanalysis Science Division (837.03)	
NIST Research Advisor: Dr. James Batteas	
Title of Talk: Preparation and Characterization of Proteins and Hybrid Lipid Bilayers on Gold Surfaces	

Abstract of Talk:

Assembly of proteins on surfaces can provide a means of developing sensing technologies. However, as the organization of the protein on the surface can influence its structure and efficacy for binding, methods of organizing proteins in selective configurations at specific sites on surfaces are required. In addition to investigate inherent protein function when organized on surfaces, a native environment must be provided to model the typical lipid bilayer structure. In this project we have focused on two main components: 1) patterning of proteins for selective binding and 2) measurements of the structure and stability of hybrid lipid bilayers as a membrane mimetic. In the first part, glucose thiols have been patterned on surfaces to examine their selectivity for binding to Concavalin A. In the second part, a hybrid bilayer has been constructed which can be employed to provide a test-bed for the assembly of proteins. Both of these systems have been characterized by atomic force microscopy (AFM) to examine their detained nanostructure and thermal-mechanical stability.

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August 10 – 12, 2004

Name: Debra Lauterbach	**Grant Number:** 70NANB4H1060
Academic Institution: Iowa State University	**Major:** Computer Engineering
Academic Standing as of September '04: Sophomore	
Current Career Plans: I would like to go to graduate school in Human-Computer Interaction.	
NIST Laboratory, Division and Group: Information Technology Laboratory, Information Access Division, Visualization and Usability Group	
NIST Research Advisor: Dr. Emile Morse	
Title of Talk: Adding Speech to Text Transcription to a Video Annotation Tool	

Abstract of Talk:

Usability testing at NIST consists of the monitoring and recording of analysts as they interact with a piece of software. During the testing, the subject is encouraged to use verbal protocol, which is a method of getting the user to talk aloud about what they are thinking and problems they may be having. These audio comments are recorded, along with video screen capture of the computer display. Currently, there is no automated way for usability engineers to transcribe these very useful audio comments, which are typically several hours in length.

The desired solution to this problem is to create a transcription that would automatically index into the video. That way, it would be possible to search for keywords about problems the user experienced, and bring up the corresponding video to see what task the user was attempting to do at that time. To achieve this solution, I created a C++ Windows dialog-based program that has the capability of implementing IBM's ViaVoice speech recognition engine and producing a transcript of the audio. The transcript includes timestamps of the start and end times for each phrase in the recording; this way, once the transcript is inserted into a database, all query results will include precise timing information.

There are several challenges to speech recognition, most important of which is the accuracy of the transcription. I conducted several studies on previous audio data to determine the WER (Word Error Rate) of transcriptions and the factors that could reduce error, such as using filters to erase background noise. In addition, we wanted to test the accuracy of the software on audio from a simulated usability test. To do this, I conducted a user experiment in which participants were asked to use verbal protocol while performing a task, and also read a script out loud. The results helped to show the differences in WER between extemporaneous speech and prepared speech, and demonstrated the feasibility of using the transcriptions for analytical purposes.

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August 10 – 12, 2004

Name: Michael V. Le	**Grant Number:** 70NANB4H1055
Academic Institution: University of California, Irvine	**Major:** Information and Computer Science
Academic Standing as of September '04: First Year Graduate Student	
Current Career Plans: Plan to pursue a PhD in computer science at UCLA.	
NIST Laboratory, Division and Group: Information Technology Laboratory, Software Diagnostics and Conformance Testing Division, Test Method Research Group	
NIST Research Advisor: Christopher Dabrowski	
Title of Talk: Investigating Reliability Characteristics of Medium-Sized Service-Oriented Architectures	

Abstract of Talk:

The ability to detect and adapt to failures is vital to any service-oriented computing system. There are currently many service-oriented systems deployed using a wide range of different topologies for service composition and failure detection and recovery mechanisms. Different topologies have different access patterns and behaviors that can affect the effectiveness of the failure detection and recovery mechanism employed. Although there have been extensive research in failure detection and recovery mechanisms for distributed applications, little is known about how these mechanisms will behave relative to different service composition topologies.

In this project, we analyze the reliability characteristics of different software composition topologies with respect to a failure detection and recovery mechanism found in SLP (Service Locator Protocol). We focus on three general service-oriented topologies: hub and spoke, sequential, and hierarchical. Our project consists of simulating the behaviors of the three service-oriented topologies on top of an existing simulated instantiation of SLP. A series of test is run for each of the three topologies with varying degrees of service failure. Service can fail at anytime and the application must detect and recover from such failure based on the behavior described in its architecture. The three measurements we use to determine the reliability characteristics of the different service-oriented topologies are the time required to complete the task, the functional effectiveness (the proportional amount of time the application has all the services it needs to accomplish a task), and the total number of messages necessary to complete the task. We postulate that the software topology that most naturally lends itself to efficiently detect execution progress will be the most successful in completing its task in the shortest amount of time and using the least amount of messages. We hope that the results from these experiments will greatly help the standards developers and application designers in understanding reliability of service-oriented architectures.

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August 10 – 12, 2004

Name: Constance P. Lee	**Grant Number:** 70NANB4H1032
Academic Institution: Northwestern University	**Major:** Materials Science and Engineering
Academic Standing as of September '04: Junior	
Current Career Plans: Intentions to continue studies in Graduate School	
NIST Laboratory, Division and Group: Materials Science and Engineering Laboratory, Ceramics Division	
NIST Research Advisor: Dr. John E. Blendell, Dr. Adam Scotch	
Title of Talk: Grain Growth and Boundary Migration in Strontium Titanate	

Abstract of Talk:

The properties of a polycrystalline material are usually considered to be determined mainly by the composition (phase, phase distribution, etc.) and microstructure (grain size, porosity, etc.). However most materials are inhomogeneous and anisotropic: not all grains are uniformly sized or randomly oriented throughout the crystal and the material properties vary with crystal orientation and sample direction. It is important to understand how basic micro-structural changes during grain growth and boundary migration can be influenced to produce desired microstructures and thus optimum properties.

Strontium Titanate, ($SrTiO_3$), was chosen as a model material for a study of grain boundary migration. Single crystal seeds of $SrTiO_3$ of known orientations were imbedded into polycrystalline material ($SrTiO_3 + xTiO_2$) containing random grain orientations. The single crystal seeds were grown into the polycrystalline matrix and can be viewed as very large grains that provide many interfaces with the polycrystal. Analysis of a large number of interfaces increases the precision of the data.

Two sets of samples, each containing 0%, 1%, and 5% (by volume) excess TiO_2, which forms a liquid phase at the sintering temperature, were examined; one sintered at 1500°C for four hours in air and another sintered in a reducing atmosphere of Ar with 5% H_2. Previous observations had shown that the presence of the TiO_2-rich liquid phase resulted in greater seed growth and smaller matrix grains as compared with the samples without any excess TiO_2. The presence of a liquid phase combined with the reducing atmosphere resulted in abnormal grain growth (exaggerated growth of a few large grains in the matrix).

Orientation mapping of the interfaces between the single crystal and polycrystal is being conducted on the samples to quantitatively study the effect of grain misorientation on grain boundary migration. Using a scanning electron microscope (SEM) and electron back-scattered diffraction (EBSD), it is possible to rapidly determine and map the orientation of all the grains on large areas of a sample. Subsets of grains in the maps have been isolated and pole figures generated and used to determine if there is a misorientation relationship among the grains touching the interface of the single crystal as compared to the matrix grains. The hypothesis is that specific grain orientations will be absent from the set of interface misorientations to indicate that the single crystal grows more rapidly into grains of these misorientations.

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August 10 – 12, 2004

Name: Jonathan Lee	**Grant Number:** 70NANB4H1045
Academic Institution: University of California, Berkeley	**Major:** Engineering Physics
Academic Standing as of September '04: Junior	
Current Career Plans: Plan to earn a Ph.D. in Mechanical Engineering.	
NIST Laboratory, Division and Group: Manufacturing Engineering Laboratory, Precision Engineering Division, Surface & Microform Metrology Group	
NIST Research Advisor: Theodore V. Vorburger & Joseph Fu	
Title of Talk: Eliminating Rotational Errors in C-AFM's 6-axis Stage	

Abstract of Talk:

At NIST, we have a six-axis stage for our Calibrated-Atomic Force Microscope (C-AFM). The C-AFM is an atomic force microscope with three measuring axes directly linked to laser interferometers. It is capable of measuring with sub-angstrom resolution in the Z-axis. The stage can move in three translation directions (x,y,& z) and three rotation directions (roll, pitch, & yaw) by using seven PZTs (piezoelectric translators). Though the C-AFM is only required to translate in the three directions while taking measurements, rotation of the stage is necessary to compensate for any unwanted motions. Therefore, along with the six-axis stage, there is a controller that continually monitors its motion using capacitive position sensors. The controller uses a feedback loop to readjust the rotations in each axis; as the sensors read a rotational displacement, the controller will command certain PZTs to counteract that displacement. The company that manufactures this controller specifies a certain amount of accuracy for the rotational compensation. In other words, for every 100 microns of translation (in any direction), there can only be about a tenth of a micro-radian of rotation (around any axis).

Last summer, it was detected that the controller was not sufficiently compensating for several rotations. My task was to recalibrate the controller to within specification and test for repeatability and reproducibility. In my talk, I will discuss the set up of the stage, the procedure of my experiments, and the analysis of my data. Adjustments to a list of hundreds of parameters were made slowly and methodically. Ultimately, we achieved a set of parameters that satisfactorily eliminates rotations. I will finally discuss the statistical analysis that I performed to ensure the repeatability and reproducibility of each rotation measurement.

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August 10 – 12, 2004

Name: Jennifer M. Lenkner	**Grant Number:** 70NANB4H1028
Academic Institution: College of Mount St. Joseph	**Major:** Chemistry
Academic Standing as of September '04: Senior	
Current Career Plans: Plan to go to graduate school to pursue studies in chemistry	
NIST Laboratory, Division and Group: Electronics and Electrical Engineering Laboratory, Semiconductor Electronics Division	
NIST Research Advisor: Dr. Darwin Reyes-Hernandez	
Title of Talk: Development, Fabrication, and Characterization of Novel Electrodes for Use as Cell Based Sensors	

Abstract of Talk:

Cell based sensors (CBS), in which living cells and electronics are combined, promise tools capable of rapid detection of cellular responses to biological and chemical stimuli. Such stimuli could be directed independently to single cells or to small groups of cells when enclosed in a microfluidic network. In order to assess responses from single cells or from small groups of cells the fabrication of micron-size electrodes on or close to biocompatible materials is needed. Previous efforts in our lab to pattern small groups of cells have shown successful results when cells were patterned on PEMs (polyelectrolyte multilayers) adsorbed on polydimethylsiloxane (PDMS). In this work, the fabrication and characterization of gold electrodes of various dimensions on PDMS surfaces was investigated. The surface characteristics and morphology were explored using AFM and the functionality of the electrode examined through electrochemical studies. It was found that the surface of the electrodes was riddled with wrinkles. These wrinkles resemble trenches or channels and have depths in the order of hundreds of nanometers. Despite the rough surface of the gold film and due to its apparent continuity, the electrodes performed well in electrochemical studies and may be suitable for measurements on the single cell level.

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August 10 – 12, 2004

Name: Claire V. Lewinger	**Grant Number:** 70NANB4H1017
Academic Institution: University of Florida	**Major:** Civil Engineering (Structures)
Academic Standing as of September '04: Graduate Student First Year	
Current Career Plans: I plan to complete my Master's Degree in December 2005, and go to work as a Structural Engineer in a design firm.	
NIST Laboratory, Division and Group: Building and Fire Research Laboratory, Fire Research Division, Analysis and Prediction Group	
NIST Research Advisor: Dr. Kuldeep Prasad	
Title of Talk: A Study of the Effect of Fire on Steel Framed Buildings	

Abstract of Talk:

It is of great concern to investigate the effects of an intense fire on the structural stability of a steel frame. Testing the validity of results from temperature loads will prove paramount in deciding whether any software package can be confidently used to analyze steel frames in high temperature situations.

The goal of the research is to determine whether SAP2000 can produce accurate results from thermal loading. This way, the structural responses of fire events along with (possibly) extreme loading can be viewed. Some nonlinear structural analysis packages, such as Abacus and ANSYS, can be used to view results from thermal loading, but those programs are expensive and time consuming. SAP2000 is a widely used linear analysis and design software package that produces results quickly and inexpensively.
To begin the research, I had to learn how to use SAP and understand its output and results. Then a simple three-story model was chosen to verify the results from SAP. What was important to learn is that SAP has the capability to calculate thermal expansion as temperature increases, but does not account for material changes and degradation. Given this important result, it became necessary to bypass the graphical user interface and manually input material properties for members as temperatures increased. The presentation will include results from SAP as temperature increases including the viability of using SAP in the future to model complex frames under fire loading.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Stephen Lin	**Grant Number:** 70NANB4H1062
Academic Institution: University of Pennsylvania	**Major:** Electrical Engineering
Academic Standing as of September '04: Sophomore	
Current Career Plans: Plan to go to graduate school to pursue studies in electrical engineering	
NIST Laboratory, Division and Group: Electronics and Electrical Engineering Laboratory, Semiconductor Electronics Division, Metrology for System-on-Chip Group	
NIST Research Advisor: Dr. Allen R. Hefner, Dr. M. Yaqub Afridi	
Title of Talk: Thermal Characterization of Microhotplate Devices and Gas-Sensor System-on-a-Chip (SoC)	

Accurate temperature measurement of the microhotplate devices used in a gas-sensor system-on-a-chip is essential for gas classification/quantification and optimal operation of the system. Thermal characterization of these microhotplate devices allow for precise control of heating.

In the work described here, a fully automated thermal characterization method was developed and implemented to characterize the microhotplate-based gas-sensors. Four computer programs were developed and written using the Labwindows/CVI programming environment to control instruments through a GPIB computer interface. These programs measure the TCR (temperature coefficient of resistance) value of the polysilicon material, the thermal efficiency of the microhotplate, the polysilicon resistance drift, and the DC response of the gas-sensor.

The microhotplate uses a polysilicon heating element. The TCR of the polysilicon heater material used in the AMI CMOS foundry process was measured and found to be approximately 1.02×10^{-3}/ °C. The thermal efficiency of the microhotplate's polysilicon heater was measured and found to be about 21°C/mW at an operating temperature of 300°C. It was observed that the resistance of the polysilicon heating element drifts at high temperatures over an extended period of time. In the future, the thermal characterization method described here will be used to profile and evaluate new gas-sensors.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Paul William Matthews	**Grant Number:** 70NANB4H1067
Academic Institution: Coppin State University	**Major:** Computer Science

Academic Standing as of September '04: First year graduate student at University of Maryland College Park

Current Career Plans: I plan to complete my graduate school education, obtain a Masters degree in Information Management, and pursue a career committed to researching Computer Forensics.

NIST Laboratory, Division and Group: Information Technology Laboratory, Computer Forensics, National Software Reference Library Group

NIST Research Advisor: Mr. Douglas White

Title of Talk: Reducing NSRL Overhead: Finding Similar Attributes in Multiple Language Versions of Microsoft Windows' Internet Files

Abstract of Talk:

The Information Technology Laboratory's Computer Forensics department endeavors to collect all forms of commercial software by storing purchased or donated software packages into the highly effective National Software Reference Library (NSRL). Hash computations on NSRL yield uniquely identifying signatures (called SHA-1s) for each file that compose the software; those signatures are stored in a database known as the Reference Data Set (RDS), which is very valuable. For example, if just one change, such as an additional space or line break, is added to a file its newly hashed signature will not match its original signature. This feature allows researchers to determine whether users have altered commercial product files. RDS is currently being used primarily by Law Enforcement to minimize the search criteria of seized computers and to determine what files are necessary for evidence.

Because NSRL must uniquely identify each file (and each version of each file) the capacity to store different language versions of the same software (i.e. Windows XP English, Windows XP Dutch, Windows XP Arabic) can reach its climax in purchasing cost, processing time, and storage space. Therefore, this research is particularly concerned with finding a set of attributes consistent across various language versions of Microsoft Windows' internet (HTML) files. Once the set of consistent attributes are found, they can be stored and hashed; thus allowing RDS to derive one digital signature that serves as the identifying mark for multiple language versions of the same file thereby reducing overhead incurred by the department.

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NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Brenna M. McGruder	**Grant Number:** 70NANB4H1040
Academic Institution: Mississippi State	**Major:** Biochemistry and Molecular Biology
Academic Standing as of September '04: Senior	
Current Career Plans: Graduate school to purse a PhD and then either academia or R and D	
NIST Laboratory, Division and Group: Chemical Sciences and Technology Laboratory, Biotechnology Division, DNA Technology	
NIST Research Advisor: Dr. John Jakupciak	
Title of Talk: Real-Time Measurements for Cancer Detection using Telomerase	

Abstract of Talk:

In normal cells telomeric DNA sequences are degraded with each cell division. In gametes and cells no longer responsive to growth controls this means the activation of telomerase to maintain their telomere length. With 85% of cancers being telomerase positive, telomerase would be an impressive biomarker of early cancer and possible approach to therapeutic strategies. Currently there are no high-throughput or robust methods to easily and economically test for telomerase enzyme activity in the body. As a part of the National Cancer Institute Early Detection Research Network, we have developed a Real-Time Taqman assay as a potential method of early cancer detection and successful use of telomerase as a biomarker. The Real-Time Taqman assay is high-throughput, timely, and economical in comparison to the current accepted methods of analysis. Using human lung carcinoma extracted through multiple techniques we will also show that our assay has a high level of detection, enough to detect telomerase despite the extraction method. With this Real-Time assay the extraction method is no longer critical, and the high level of detection should prove worthwhile in clinical diagnostics and research studies.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Kelly McQuighan	**Grant Number:** 70NANB4H1002
Academic Institution: Rice University	**Major:** Physics
Academic Standing as of September '04: Junior	
Current Career Plans: Undecided	
NIST Laboratory, Division and Group: Physics Laboratory, Ionizing Radiation Division, Radiation Interactions and Dosimetry Group	
NIST Research Advisor: Dr. Michael Mitch	
Title of Talk: Automation and Testing of a New Plastic Scintillator Dosimeter for Radioactive Sources Used in Prostate Cancer Brachytherapy	

Abstract of Talk:

Brachytherapy is an internal radiation therapy technique for treating cancer that involves placing a radiation source either close to or inside a tumor. Brachytherapy for prostate cancer involves the implantation of 80 to100 small sealed radioactive sources called "seeds" in the prostate gland. One major advantage of this therapy is that the sources, which emit low-energy x-rays, deliver maximum dose to the cancer cells while minimally impacting the surrounding tissue.

NIST has calibrated 31 different seed models made by 18 different companies. Task Group 43 (TG43) of the American Association of Physicists in Medicine (AAPM) has issued a series of papers including general dosimetry formulas as well as axial dose and anisotropy consensus data sets for various seed models. Dosimetric data has traditionally been compiled from two sources: experimental measurements using thermoluminescent dosimetry (TLD) chips in plastic "solid water" phantoms and theoretical Monte Carlo calculations. Both methods have limitations. The use of solid water phantoms, which have similar radiation absorption and scattering properties to those of water, requires corrections to be made to determine the dose to liquid water, the medium of interest in medical dosimetry. In addition, inner chips may shield the outer chips from maximum exposure. Therefore, there are limits on the location of the closest chip to the seed and the minimum allowable distance between chips. In addition, the use of TLD chips requires a large integration time to acquire precise data. While Monte Carlo calculations do not have physical limits, they rely on idealized models of seed structure.

A recent grant through NIST's Small Business Innovation Research (SBIR) Program funded the development of a plastic scintillator dosimeter that measures absorbed dose in water with high spatial resolution in real time from prostate brachytherapy seeds. This new plastic scintillator dosimeter has fewer of the disadvantages of the TLD chips. To test this new instrument, data were collected for the axial dose and anisotropy tests on different seed models and the results were compared to TG43 consensus data. In addition, a computer program was developed that automates the motion of the device and data collection for the axial dose and anisotropy tests and integrates the TG43 formalism for direct comparison to published data from other seed models. The instrument is now ready to be used for measurements of new seed models.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Nathan J. Mesick	**Grant Number:** 70NANB4H1034
Academic Institution: Rensselaer Polytechnic Institute	**Major:** Mechanical Engineering
Academic Standing as of September '04: Sophomore	
Current Career Plans: Plan to go to graduate school to pursue studies in mechanical engineering.	
NIST Laboratory, Division and Group: Materials Science and Engineering Laboratory, Metallurgy Division, Materials Structure and Characterization Group	
NIST Research Advisor: Dr. Carelyn E. Campbell	
Title of Talk: Diffusion in Nickel-Base Superalloys and Bond Coats	

Abstract of Talk:

Nickel-base superalloys are known for their high temperature strengths and their corrosion resistant properties. To increase the service temperatures of the Ni-base superalloys, thermal barrier coatings (TBC) are used in conjunction with a bond coat. The role of the bond coat is to prevent diffusion between the superalloy and the TBC, especially the depletion of Al from the superalloy. Diffusion studies between various bond coat materials and Ni-base superalloys were conducted for two purposes: (1) to better understand the interaction between the bond coats and the superalloys and (2) to provide data to evaluate the current diffusion mobility database. Superalloys considered in this study were Inconel X-750, Inconel 625, Inconel 718, and CMSX-4. Bond coatings considered were RuAl, PtAl, and Ni. Diffusion couples were heat treated at 1150 C and 850 C for various times. For Ni/superalloy couples, diffusion simulations using multicomponent thermodynamics and diffusion mobility databases were performed.

Evaluation of the bond coats and the diffusion mobility database required measurement of phase fraction and composition profiles. Optical metallography and image analysis software were used to measure the phase-fraction profiles. Electron diffraction spectroscopy (EDS) was used to measure the composition profiles. This data was used to determine how well the bond coatings limited diffusion of Al out of the superalloy and into the bond coat. Comparison of the measured and calculated composition profiles and phase fraction profiles indicated whether specific mobility parameters or thermodynamic descriptions should be re-evaluated.

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NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Andrew C. Milliken	**Grant Number:** 70NANB4H1049
Academic Institution: University of Maryland	**Major:** Fire Protection Engineering
Academic Standing as of September '04: Junior	
Current Career Plans: Plan to establish a career directly linking both the fire service and fire protection engineering field.	
NIST Laboratory, Division and Group: Building and Fire Research Laboratory, Fire Research Division, Fire Fighting Technology Group	
NIST Research Advisor: Mr. Daniel Madrzykowski	
Title of Talk: Wireless Telemetry for Fire Research and Fire Service Applications	

Abstract of Talk:

Each year over a 100 fire fighters die while serving in the line of duty. Even to this day, fire fighter accountability and wellbeing while working in these hazardous environments remains at the forefront of fire fighting safety. As the use of Personal Alert Safety System (PASS) devices has become more common and detailed, the need for additional mobile transmission of information becomes necessary to paint a clearer picture of the incident and it's hazards. Currently the best method of gathering this or other fire data, even within the laboratory setting such as at NIST, requires tedious and time consuming work connecting numerous wires and cords to nearby acquisition and recording systems. In addition, fire research technologies have held a limited range of operation and flexibility as similar issues constrain testing. A rising solution to both of these issues may arrive in the form of an ultra-wideband, wireless telemetry system.

Over the past few months the effectiveness and efficiency of a wireless telemetry system has been compared, challenged and explored. Coupled with an introduction to basic fire research procedures, the telemetry system was compared to a standard wired system in a variety of examinations including calibration tests, a small room flashover burn and large two-car garage burn. In addition, initial geographical testing was completed to establish a judgment for the range of the system and potential obstacles. Finally, significant effort was applied towards verifying the precision, accuracy and possible time delays of the wireless system output to actual data. Collaboration of observed data initiated a basis and direction to the capabilities, questions and future possibilities of a detailed information gathering system for fire research and fire service applications.

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NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Van Molino	**Grant Number:** 70NANB4H1052
Academic Institution: Princeton University	**Major:** Mathematics
Academic Standing as of September '04: Senior	
Current Career Plans: Go to graduate school and then do research and teach at the university level.	
NIST Laboratory, Division and Group: Information Technology Laboratory, Statistical Engineering Division	
NIST Research Advisor: Andrew Rukhin, Stefan Leigh	
Title of Talk: Markov Chains and MCMC Methods	

Abstract of Talk:

The concept of a Markov chain was introduced in 1906 by A. A. Markov. The usefulness of the Markov chain as a modeling tool was quickly realized and by the 1960's so much work had been done that many considered the field to be an unlikely source of new research. However, when Markov chain Monte Carlo (MCMC) algorithms were introduced, the field enjoyed a spectacular revival and exciting new work is being done using MCMC in many different disciplines ranging from mathematical logic to ecology.

Because of their wide applicability, my advisors and I have developed a two-day course on these topics that will be taught to NIST scientists in late August. The first day will cover Markov chain theory, which is both powerful in its own right and should be understood in order to utilize MCMC algorithms intelligently. The second day will cover MCMC methods and some of the interesting problems to which these methods have been applied.

This talk will survey some basic Markov chain theory, emphasizing the theory's versatility by applying it to several simple problems in different fields of study. MCMC methods will be introduced briefly. To illustrate the power of these simulation tools, this talk will discuss how this machinery can be applied to the satisfiability problem of mathematical logic, a famous problem shown to be NP-complete by Stephen Cook in 1971.

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NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Eric J. Montgomery	**Grant Number:** 70NANB4H1043
Academic Institution: University of Maryland, Baltimore County	**Major:** Physics and Optical Engineering
Academic Standing as of September '04: Senior	
Current Career Plans: Plan to go to graduate school to pursue studies in physics.	
NIST Laboratory, Division and Group: Physics Laboratory, Optical Technologies Division, Optical Thermometry and Spectral Methods Group	
NIST Research Advisor: Dr. Alan Migdall	
Title of Talk: Exciting Frontiers in Single Photon Counting Detectors	

Abstract of Talk:

The continued advancement of single-photon counting detectors (SPDs) in the infrared has exciting applications, from quantum computing to correlated photon quantum cryptography, and even to technical applications such as advanced single transistor analysis of prototype CPUs. The most efficient infrared SPDs yet developed are based on avalanche photodiodes (APDs), which use a short (~1 ns) electrical pulse to bias the photodiode above its breakdown voltage. During this window, photons incident on the APD create electron-hole pairs, and the resulting avalanche of breakdown electrons is detectable by sophisticated electronics.

In the spirit of advancing SPD research, we conduct calibrations of APD detection efficiency (# photons detected / # photons incident) using both conventional and quantum correlated photon methods. Conventional methods involve careful calibration of a pulsed laser source's intensity with standard semiconductor photodiodes, and then calibrated attenuation of the source to arrive at a low-intensity, well-characterized source suitable for APD calibration. The downside of this technique is that it relies on the calibration of the series of attenuators used. Correlated photon methods, on the other hand, provide an independent calibration technique; this is based on the process of parametric down-conversion (PDC). PDC occurs when photons pass through an appropriate nonlinear crystal and decay into correlated photon pairs, exiting the crystal at different angles than the input beam. Conservation of energy and momentum must hold, and use of such "phase-matching" equations allows the direction, polarization, and wavelength of one output photon beam to be determined if the second beam is measured. The calibration of APDs places a detector under test (DUT) in one correlated photon beam, and a second, also uncalibrated SPD in the other correlated photon beam. The second SPD is the so-called "herald" detector, and announces the imminent arrival of one of a pair of correlated photons to the DUT. Every time the herald announces such an event, the DUT is measured to see if a photon has been detected, and the ratio of DUT detection events to herald events provides an absolute, independent measure of the detection efficiency of the DUT.

Our experiments allow both methods of APD calibration to be carried out and compared. This summer our lab group has worked towards bringing the quantum correlated photon method to the 0.1% level of precision, and has also successfully characterized a prototype infrared SPD from IBM with the conventional method of calibration.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Miguel A. Morales	**Grant Number:** 70NANB4H1046
Academic Institution: University of Puerto Rico at Mayaguez	**Major:** Theoretical Physics and Computer Science
Academic Standing as of September '04: Graduate Student	
Current Career Plans: Obtain a Ph.D. in Theoretical Condensed Matter Physics.	
NIST Laboratory, Division and Group: Physics Laboratory (PL), Electron and Optical Physics Division	
NIST Research Advisor: Dr. Charles W. Clark	
Title of Talk: Phase Diagram of a Gas of Atomic Bosons, Atomic Fermions, and Heteronuclear Molecules	

Abstract of Talk:

Recent advances in cooling techniques have made it possible to cool dilute atomic gases to quantum degeneracy: a temperature regime where quantum effects determine the behavior of the system. When degeneracy is reached, new phenomena occur such as Bose-Einstein condensation and condensation of pairs of fermionic atoms.

These gases present us with an invaluable tool in the study of quantum phenomena, as it is possible to control not only the magnitude of atomic interactions, but also whether those interactions are attractive or repulsive. This control over atomic interactions allows experimentalists to "change" the system from a gas of free ultra-cold atoms to a gas of loosely bound molecules, created by the resonant coupling of a bound molecular state with a free atomic scattering state, known as a Feshbach resonance. Very recently, scientists at JILA and MIT discovered the existence of Feshbach resonances between atoms of different species. This discovery opened up the possibility of creating ultra-cold heteronuclear molecules composed of fermionic and bosonic atoms.

We present a study of the phase diagram of an ideal gas mixture of fermionic and bosonic atoms and fermionic molecules, in thermal and chemical equilibrium. The molecules have an adjustable internal energy resulting from the existence of an interspecies Feshbach resonance between fermionic and bosonic atoms. We also identify a new mechanism for cooling. A study of this ideal system can give us a good qualitative understanding of the equilibrium properties and the transition temperatures of the real system.

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NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Katherine E. Myers	**Grant Number:** 70NANB4H1003
Academic Institution: Lebanon Valley College	**Major:** Physics
Academic Standing as of September '04: Senior	
Current Career Plans: Plan to go to graduate school to pursue studies in Physics	
NIST Laboratory, Division and Group: Physics Laboratory, Optical Technology Division, Laser Applications Group	
NIST Research Advisor: Dr. Jeeseong Hwang	
Title of Talk: Dynamic Imaging of Lipid Bilayers on Chemically Modified Surfaces	

Abstract of Talk:

Phospholopids are the key component of cell membranes and therefore the study of phospholipid bilayers on biocompatible substrates provides key insight into how cells interact with culture substrates. To probe such interactions, we studied dimyristoyl-glycero-phosphocholine (DMPC) bilayers tagged with dihexadecyl-tetramethylinedo-carbocyanine-perchlorate ($DiIC_{16}$). The diffusion dynamics of the DMPC bilayers were investigated on various chemically modified glass coverslips, including self-assembled (SA) aminopropyl-triethoxysilane (APTES) monolayer, and SA APTES monolayers onto which proteins were micropatterned.

A polydimethylsiloxane (PDMS) stamp containing ten 30-micron wide channels was used to achieve a partial coverage of proteins on an APTES functionalized glass coverslip. A goat anti-rabbit antibody fluorescently labeled with fluorescein-isothiocynate (FiTC) was introduced to the channels and crosslinked to the APTES monolayer via glutaraldehyde. Varied antibody concentrations were used to investigate the effects of protein concentration on bilayer diffusion through the channels.

A mercury arc lamp was used for excitation and fluorescence emission was captured using a charge coupled device (CCD) camera. The diffusion constant was calculated by measuring the change in area of the bilayer as a function of time. A discussion of these analytical methods and a comparison of the diffusion constants on the various surfaces will be outlined in this talk.

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NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Jessica L. Naff	**Grant Number:** 70NANB4H1039
Academic Institution: Appalachian State	**Major:** Chemistry w/ Concentration in Forensic Science

Academic Standing as of September '04: Senior

Current Career Plans: Plan to attend graduate school to pursue studies in forensic science.

NIST Laboratory, Division and Group: Building and Fire Research Laboratory, Fire Research Division, Fire Fighting Technology Group—in conjunction with Electronics and Electrical Engineering Laboratory, Office of Law Enforcement Standards

NIST Research Advisor: Mr. Daniel Madrzykowski

Title of Talk: Re-creation of Accelerant Burn Patterns on Carpet Using the Fire Dynamics Simulator

Abstract of Talk:

In an effort to improve the scientific technology behind fire investigation as well as the validity of expert testimony given by arson investigators in court, a series of full-scale fire experiments were completed and compared to computer simulations, focusing on the ability of the model to accurately reproduce burn patterns resulting from spill fires on carpet. Using NIST's Fire Dynamic Simulator (Version 4), a computer model that mathematically calculates the physical and chemical dynamics of a fire, full-scale rooms were modeled and spill fires were re-created based on experimental and empirical values. Smokeview, a scientific visualization program then utilized FDS calculation results to develop animated simulations of the fires.

Full-scale experiments were conducted in a former military dormitory in Myrtle Beach, South Carolina. During the tests, approximately 1000 mL of gasoline was mechanically poured onto carpets and then ignited. The resulting burn patterns were then measured, photographed, and documented. It was noticed that the swirl direction and/or shape of the burn pattern was dependent on the placement of the door relative to the location of the gasoline spill. It was also observed that as the fire grew it tended to lean away from the door. Using specific inputs to account for the dimensions and material properties of the room, the area of spill, and the type of carpet in the room, the Fire Dynamics Simulator appeared to reproduce an accurate burn pattern. Thus, a good comparison between full-scale fire tests and computer models was established, further validating the ability of NIST's FDS and Smokeview programs to accurately reproduce and display a variety of real-life fire situations.

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August 10 – 12, 2004

Name: Bryan I. Nishimoto	**Grant Number:** 70NANB4H1055
Academic Institution: University of California, Irvine	**Major:** Mechanical Engineering
Academic Standing as of September '04: Super Senior	
Current Career Plans: Plan to go to graduate school to pursue Ph. D. in Mechanical Engineering	
NIST Laboratory, Division and Group: Materials Science and Engineering Laboratory, Polymers Division, MALDI-TOF-MS Methods Group	
NIST Research Advisor: Dr. Michelle Byrd	
Title of Talk: Method Development for the Preparation and Analysis of Polymer Samples Using MALDI-TOF Mass Spectrometry	

Abstract of Talk:

Polymer applications flourish in our modern world. To manufacture polymers with optimum performance properties, information about the mass distribution and chemical composition is vital. Matrix Assisted Laser Desorption Ionization Time of Flight (MALDI-TOF) mass spectrometry provides a method to determine this information accurately and easily. MALDI does not require large samples in order to function properly, and can be used for large molecules. This makes it an excellent way to analyze polymers. However, factors such as sample preparation and introduction, data processing, and instrument parameters significantly influence the outcome of a MALDI-TOF investigation. Examining and optimizing these elements require empirical analysis over a large sample space. The goal of the research is to integrate a high-throughput MALDI sample preparation station, a commercial automated data collection MS, and a semi-automated in-house data processing software into a single, self-operated three stage platform. The data collected from this setup will help to identify the optimal setup for data collection from a polymer sample via MALDI-TOF mass spectrometry and to determine consistent and optimum procedures for handling the data. This presentation will cover my contribution to this project, the data analysis front.

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August 10 – 12, 2004

Name: G. Barratt Park	**Grant Number:** 70NANB4H1056
Academic Institution: Davidson College	**Major:** Chemistry
Academic Standing as of September '04: Junior	
Current Career Plans: Plan to go to graduate school to pursue studies in physical chemistry.	
NIST Laboratory, Division and Group: Chemical Science and Technology Laboratory, Physical and Chemical Properties Division, Experimental Kinetics and Thermodynamics Group	
NIST Research Advisors: W. Sean McGivern, Jeffrey Manion, and Wing Tsang	
Title of Talk: High-Temperature Unimolecular Isomerization Kinetics of 1,4-Pentadiene	

Abstract of Talk:

Isomerizations of unsaturated hydrocarbons are a particularly interesting class of reactions important to combustion side-product formation. Highly unsaturated hydrocarbons are often formed under severe pyrolytic conditions such as those found in fuel-rich combustion regions of flames. Reactions of these molecules may play a significant role in the formation of aromatics and soot particles. Specifically, highly unsaturated diradical species have been implicated as possible intermediates in reactions leading to aromatics (1). Unimolecular isomerization of 1,4-pentadiene is therefore of particular interest because it is believed to involve diradical intermediates.

1,4-Pentadiene isomerization and decomposition was investigated in single pulse shock tube experiments at temperatures ranging from 1000-1300 K. The products were analyzed using gas chromatography. Rate parameters were derived from product concentrations. A number of parallel decomposition and isomerization channels were found to be important. However, all major identified products came directly from 1,4-pentadiene. No secondary reactions were observed. Preliminary evaluations of rate expressions for the most important isomerization reactions are as follows:

k(1,4-pentadiene → cyclopentene) = 4.3×10^{13} exp (-27574 +/- 900 K/T) s^{-1}
k(1,4-pentadiene → *cis*-1,3-pentadiene) = 4.4×10^{11} exp (-31997+/- 900 K/T) s^{-1}
k(1,4-pentadiene → *trans*-1,3-pentadiene) = 2.9×10^{15} exp (-27574 +/- 900 K/T) s^{-1}

The decomposition processes involved both homolytic bond scission and retroene reactions. The rate expression for the latter is

k(1,4-pentadiene → acetylene + propene)= 3.9×10^{12} exp (-36515 +/- 900 K/T) s^{-1}

The absence of secondary reaction indicates that pathways leading to vinyl cyclopropane as a stable intermediate may be unimportant in the temperature range studied. Further investigation is being performed into the implications of this result.

1. Arrington, C. A., Ramos, C., Robinson, A. D., and Zwier, T. S. Aromatic Ring-Forming Reactions of Metastable Diacetylene with 1,3-Butadiene. *J. Phys. Chem. A.* **1998** *102*, 3315-3322.

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August 10 – 12, 2004

Name: Ileana Marquez Pazos	**Grant Number:** 70NANB4H1006
Academic Institution: Barry University	**Major:** Chemistry
Academic Standing as of September '04: Sophomore	
Current Career Plans: Plan to go to graduate school to pursue studies in chemistry.	
NIST Laboratory, Division and Group: Material Science Engineering Laboratory, Ceramics Division	
NIST Research Advisor: Dr. Terrell Vanderah and Dr. Mike Lufaso	
Title of Talk: Ternary Phase Diagram of the System Bi_2O_3-Fe_2O_3-Nb_2O_5	

Abstract of Talk:

Subsolidus phase equilibria was studied to find the ternary phase diagram of the Bi_2O_3-Fe_2O_3-Nb_2O_5 system. This system has compounds that are reported to exhibit interesting dielectric and magnetic properties. Compositions were chosen, then Bi_2O_3, Fe_2O_3 and Nb_2O_5 were accurately weighed and ground together. To equilibrate, samples were heated and ground three or more times until they were fully reacted. Between heatings, small portions of the samples were taken for x-ray powder diffraction analysis. When the x-ray powder diffraction patterns appeared unchanged, it was determined that the compounds reached equilibrium. The peaks in the patterns indicate what compounds are present in the sample. With data from several samples, regions are identified as single, two and three phased. Particularly interesting was the region of single-phase pyrochlore found near the center of the ternary diagram. One such composition was chosen and a larger batch was synthesized to measure properties. Pyrochlore, in this system, has unusual structural features. An accurate ternary phase diagram provides information to those interested in reproducing compositions found that have useful properties.

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August 10 – 12, 2004

Name: Angelica Perez-Andujar	**Grant Number:** 70NANB4H1046
Academic Institution: University of Puerto Rico-Mayagüez	**Major: Theoretical Physics**
Academic Standing as of September '04: Graduate Student	
Current Career Plans: Pursue a PhD in Medical Physics at University of Wisconsin-Madison	
NIST Laboratory, Division and Group: Physics Laboratory, Ionizing Radiation Division, Radioactivity Group	
NIST Research Advisor: Dr. Leticia Pibida	
Title of Talk: Test Report of Radiation Detectors Against the ANSI N42.32, N42.33, N42.34 and N42.35 Standards	

Abstract of Talk:

Part of the Department of Homeland Security (DHS) efforts to avoid terrorist attacks involving radioactive materials include the test of commercially available radiation detectors. To prevent the illegal handling of radioactive material, DHS needs to provide first responders, customs agents and coast guard personnel with a list of tested equipment against the ANSI Standard (N42.32-2003, N42.33-2003, N42.34-2003 and N42.35-2004) so they can purchase the right equipment for their application and warranty the necessary equipment performance. As part of this effort, the National Institute of Standards and Technology (NIST) is in charge of coordinating the test and evaluation of radiation detectors, conducted at four national labs, as well as preparing the "Test Report of Radiation Detectors Against the ANSI N42.32, N42.33, N42.34 and N42.35 Standards". This report is a compilation of all the radiation detectors tested at Oak Ridge National Laboratory (ORNL), Pacific Northwest National Laboratory (PNNL), Lawrence Livermore National Laboratory (LLNL) and Los Alamos National Laboratory (LANL) that will be use by first responders or other DHS agencies. A brief description of each detector, the manufacturer's specification and the tests results are presented in this report. Each detector was subject to different tests according to the requirements of each of the four ANSI N42 Standard. The report presents the test results so that the users can better determine the instrument needed for their particular application and environment under which the device is going to be used.

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NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Candace Pfefferkorn	**Grant Number:** 70NANB4H1047
Academic Institution: Gettysburg College	**Major:** Physics
Academic Standing as of September '04: Junior	
Current Career Plans: Plan to go to graduate school to pursue studies in physics.	
NIST Laboratory, Division and Group: Physics Laboratory, Atomic Physics Division, Laser Cooling and Trapping Group	
NIST Research Advisor: Dr. Kristian Helmerson	
Title of Talk: Nanotube Formation from Biological Membranes Using Optical Tweezers	

Abstract of Talk:

Optical tweezers are a versatile tool for the trapping of biological objects such as cells, viruses, bacteria, and even DNA. Comprised of a tightly focused laser beam, optical tweezers can trap particles that possess the correct dielectric properties on the nanometer to micrometer scale with great ease. Employing the momentum transfer of light to an object, the laser can trap particles with a force on the order of piconewtons. We create our optical tweezers by coupling an infrared laser with the appropriate optics in to the back aperture of a high-powered microscope objective.

One interesting application of the optical tweezer is the formation of nanotubes pulled from lipid vesicles that are attached to a surface. While many attempts have been made to create stable lipid nanotubes, these have proved unsuccessful due to the leaky nature of the lipid membrane. Polymersomes, made from the diblock polymer polybutadine-ethylene oxide, are much like the liposomes in that they maintain a thin and flexible membrane when mixed with a surfactant. The use of polymers with double bonds, in the core of the membrane, has the potential for cross-linking, or stiffening through chemical processes. We have successfully pulled nanotubes from polymersomes and used the cross linking process to stabilize them. We ensure the polymersomes are cross linked by puncturing holes in the otherwise stretchy, flexible, and resealable membranes with an ultraviolet laser pulse. I will present recent results on the pulling and cross-linking of polymer nanotubes and their possible uses in advancing nanotechnology and microchemical or biological transport.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Leah Pike	**Grant Number:** 70NANB4H1015
Academic Institution: Washington University in St. Louis	**Major:** Mechanical Engineering
Academic Standing as of September '04: Junior	
Current Career Plans: Mechanical Engineering PhD.	
NIST Laboratory, Division and Group: Manufacturing Engineering Laboratory, Intelligent Systems Division	
NIST Research Advisor: Dr. Nicholas Dagalakis, Dr Jason Gorman	
Title of Talk: Image Analysis of MEMS-Based Nanopositioning Stages	

Several micro-scale motion stages based on microelectromechanical systems (MEMS) technology have been designed and fabricated at NIST. These MEMS-based nanopositioners have been developed for applications in nanomanipulation and scanning probe microscopy. This presentation will concentrate on the initial characterization of these devices using imaging analysis. The main objective of the image analysis is to determine the relationship between the input voltage to the nanopositioner and the output displacement. Thermal actuators are used to drive the nanopositioners, which are known to be nonlinear. Therefore, a careful calibration of the input-output relationship is necessary for high-precision motion. In addition, a better qualitative understanding of the overall motion of the nanopositioner mechanism is required. These nanopositioners are compliant mechanisms, which have a monolithic design with flexure hinges for generating rotational motion. Therefore, as a voltage is applied to the thermal actuator, the entire structure deforms. The image analysis has been used to verify that the structure deforms as predicted by finite element analysis. Video of the deforming structure during operation will be presented along with quantitative data on the device calibration. Future plans for the use of image analysis in the characterization of these devices will also be presented.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Robert J. Radford	**Grant Number:** 70NANB4H1012
Academic Institution: University of California, Santa Barbara	**Major: Biochemistry**
Academic Standing as of September '04: Junior	
Current Career Plans: PhD in Chemistry	
NIST Laboratory, Division and Group: Physics Laboratory, Ionizing Radiation Division, Radioactivity Group	
NIST Research Advisor: Hiromu Kawoaski and Dr. Kenneth Inn	
Title of Talk:	

Abstract of Talk:

With over 70% of the earth surface covered in water, monitoring the quality of our oceans is one of the most important tasks in science today. Both Shellfish and Seaweed have been shown to be effective indicators of the levels of radionuclide such as Plutonium, Uranium and Americium to name a few.

One of the overall, goals of our group is to test various shellfish and seaweed specimen from different parts in the world for these radionuclides. Once a large sample set is collected a standard radionuclide levels in our oceans can be established. Furthermore, this standard can be used to monitor the changes in their levels for years to come.

However, a problem arose when the blank, a sample containing for shellfish or seaweed and consequently no radionuclide, began to show activity indicating contamination. These blanks are essential to the overall project because they give a baseline for comparison of the various shellfish and seaweed samples.

The project that follows is a systematical experimental set, which tries to narrow down and isolate the source of contamination from sixteen different variables that occur throughout the experimental process. The sources of contamination accounted for in the set range from, the fume hood to the glassware and reagents used. Assuming that one of the variables accounted for is indeed the source of contamination; well over 256 experiments would normally have been preformed in order to isolate the point of contamination. Since this is not an efficient use of resources, an experimental design was made using Exploratory Data Analysis (EDA).

EDA narrowed an unfeasible 256 experiments to a very manageable 32. The set is then further subdivided into 4 sets of 8, based of use of reagents. The experimental design will isolate or narrow down the source or interactions of variables of contamination in a timely and cost effective manner.

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NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Ian P. Rafferty	**Grant Number:** 70NANB4H1009
Academic Institution: St Mary's College of Maryland	**Major:** Physics
Academic Standing as of September '04: Graduated	
Current Career Plans: Plan to temporarily work on an organic garm, travel, and then go to Graduate School in Mechanical Engineering.	
NIST Laboratory, Division and Group: Building and Fire Research Laboratory, Fire Research Division, Materials and Products Group	
NIST Research Advisor: Dr. Greg Linteris	
Title of Talk: Flame Size vs. Heat Release Rates	

Abstract of Talk:

The heat release rate, which describes reaction of fuel and oxygen, is the most important parameter for determining material flammability. The cone calorimeter is a widely used, reliable, and accurate instrument for determining heat release rates of burning materials; however it is time consuming and expensive. If a cheaper and faster (and still accurate) method for determining heat release rates of burning materials could be developed, the measurement might be more widely used in fire research, and could allow for high throughput techniques.

The present approach is to use flame size as a surrogate for heat release. The cone calorimeter uses measurements of the oxygen consumption of the flame to predict heat release rates. Existing flame theory predicts that oxygen consumption is correlated with flame surface area. Therefore the heat release rate should correlate with the flame surface area. For our experiments we captured visual images of small, stable, laminar flames. The varied parameters were gaseous fuel flow rates, air co-flow rates, polymer type, and radiant flux. We then determined the flame outline data using a publicly available image analysis program, and a custom made image processing program to calculate the height, surface area, and volume from the complicated outline. To filter out extraneous light from black body soot emission and image the reaction sheet we also included zero, one, and two CH line filters in front of the cameras. Results have shown a consistent trend in comparisons between the flame area and heat release rate of gaseous, liquid, and polymer fuel samples calculated using either the cone calorimeter or based on mass loss times the heat of combustion. Using CH line filters also appears to work better than standard visual images and two filters are and improvement over one.

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NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Carmen R. Reedy	**Grant Number:** 70NANB4H1072
Academic Institution: Radford University	**Major:** Chemistry
Academic Standing as of September '04: Junior	
Current Career Plans: Plan to attend graduate school and study forensic science or analytical chemistry.	
NIST Laboratory, Division and Group: Chemical Science and Technology Laboratory, Surface and Microanalysis Science Division, Analytical Microscopy Group	
NIST Research Advisor: Jennifer Verkouteren	
Title of Talk: Investigations of Explosive Particles in Simulated Fingerprints	

Abstract of Talk:

Since September 11th there has been a heightened awareness about Homeland Security and explosives. My project deals with that exactly. The goal of the project is to develop a method to measure the total mass of explosive particles on simulated fingerprints by means of counting and sizing the particles through an imaging technique and doing a direct measurement of the mass. Once this goal is achieved it can be utilized in further research, for example to find the most efficient procedure to swipe a fingerprint. The instruments being used to achieve the aim of the project are Polarized Light Microscopy, which provides images of the fingerprint highlighting the explosive particles, and Ion Mobility Spectrometry, providing a direct measurement of the mass of explosive particles present in the fingerprint.

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NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Jenn Robinson	**Grant Number:** 70NANB4H1013
Academic Institution: Cornell University	**Major:** Physics
Academic Standing as of September '04: Senior	
Current Career Plans: Graduate school in Physics	
NIST Laboratory, Division and Group: Physics Laboratory, Atomic Physics Division, Laser Cooling and Trapping Group	
NIST Research Advisor: Dr. Trey Porto	
Title of Talk: Improving Trapping and Detection of BECs in Optical Lattices	

Abstract of Talk:

As part of the Quantum Information Project at NIST, this effort focuses on trapping cold neutral Rubidium atoms in a periodic optical potential, or optical lattice. These trapped atoms have applications as quantum bits, or qubits, as well as in modeling intractable quantum physics problems. The atoms are cooled to Bose-Einstein Condensates, and then loaded into an optical lattice for study. We have taken advantage of our recent move to improve several aspects of the experiment. Two important developments concern the production of the lattices beams and detection of the atoms in the lattice. My research focused on improving existing techniques for both of these.

The lattice potential is made from two counterpropagating laser beams, the phase differences of which affect the characteristics and stability of the lattice potential. Our lab recently started producing lattice beams using optical fibers with built in beam-splitters. While fibers produce better beam quality and more stability, low frequency noise in the fiber can cause the phase difference between the two outputs to drift over time. Using a Michaelson-Morley Interferometer created within the fiber by the built-in splitter and partial reflection off the output face, the drift of the phase was observed and correction methods were implemented.

Another challenge in our effort is measuring the state population in the BEC. Previous methods relied on repeated imaging of the BEC, which destroys each BEC that is imaged. Because this method is time-consuming, inefficient, and does not provide a dynamic picture of the state population, Faraday Spectroscopy was suggested as an alternative. Using the effects of an atom spin on the polarization of a probe beam of linearly polarized light, the state population and energy levels can be dynamically probed in a single shot and without destroying the BEC.

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NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Veronica Rodriguez-Rivera	**Grant Number:** 70NANB4H1046
Academic Institution: University of Puerto Rico-Mayaguez Campus	**Major:** Chemical Engineering
Academic Standing as of September '04: Senior	
Current Career Plans: Plan to go to graduate school to pursue studies in biomedical engineering.	
NIST Laboratory, Division and Group: Material Science and Engineering Laboratory, NIST Center for Neutron Research, Neutron Condensed Matter Science Group	
NIST Research Advisor: Dr. Susan Krueger	
Title of Talk: Phase Behavior of Mixed Lipid Bilayered System	

Abstract of Talk:

Lipid mixtures of short and long amphiphile chains self-assemble in water to form a great variety of structures. The morphology of these structures include phases composed of extended flexible bilayer membrane that may display order by stacking with a periodicity as in the anisotropic lamellar phase, or they may also form bilayered miscelles (or bicelles), bilayered disks formed of a long lipid chain with their edges stabilized by short chain lipid, with diameter of a few hundred angstroms.

The lipid mixtures have a great potential in the study of membrane proteins and peptides. These mixtures imitate the physical properties of biological membranes and they are stable over a wide range of temperatures, pH and ionic strength. By having a detailed description of the morphology of the lipid mixtures and understanding their phases will help increase their use in various structural biology techniques.

Our goal was to study the effect on transition between the bicelle to lamellar phase by changing the concentration of lipid in the solution. Each sample consisted of molar ratios of DHPC:DMPC:DMPG of 0.2:1:0.067. The concentration of lipid was of 20%, 10% and 5%. The 20% sample has a liquid to gel phase transition temperature of near 25°C. The lamellar phase forms above 25°C. By lowering the sample's concentration and by an isotropic substitution of H_2O by D_2O, we found some intriguing results: the liquid to gel phase transition and lamellar phase temperature shifted. SANS, reflectometry and crossed polarizers were use to study the transition between the bicelle to lamellar phase. With these results, the structure of the phase boundary between the bicelles and lamellar morphology was better understood and characterized.

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August 10 – 12, 2004

Name: Dorea R. Ruggles	**Grant Number:** 70NANB4B1018
Academic Institution: Gustavus Adolphus College	**Major:** Physics
Academic Standing as of September '04: Junior	
Current Career Plans: Plan to go to graduate school to pursue studies in acoustic physics.	
NIST Laboratory, Division and Group: Building and Fire Research Laboratory, Materials and Construction Research Division, Structures Group	
NIST Research Advisor: Dr. Emil Simiu, Dr. Michael Riley, Dr. William Fritz	
Title of Talk: Database-assisted Design for Structures Subjected to Wind Loads	

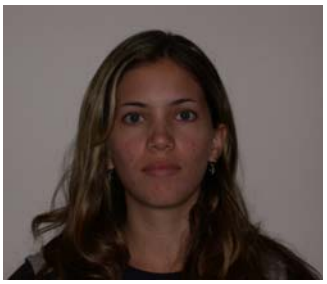
Abstract of Talk:

Wind loads specified in building codes have historically been based on measurements of peak pressures obtained from a limited number of points on a structure's envelope. However, actual wind-induced stresses in structural members are not determined by selected peaks but by pressure time histories acting over a building's entire envelope. Peak pressure measurements from individual points overestimate the wind-induced stresses, and their application results in designs that are inconsistent with respect to failure risk.

Advances in computational power now allow calculations of wind-induced stresses to be far more realistic than was ever possible before. Designers with access to millions of data points obtained in wind tunnels and compiled in aerodynamic databases are able to create designs that are both safer and more economical than in the past, an application referred to as database-assisted design. Differences between the crude estimates provided in building codes and the more accurate estimates produced by database-assisted design have recently been shown to be as high as 50 to 70%.

Confident use of aerodynamic databases is dependant on reliable wind tunnel measurements, which have not been thoroughly examined to date. In response to this need, NIST is conducting a round-robin test on a typical industrial building and comparing the resulting measurements from laboratories in Texas, Colorado, South Carolina, Canada, France, and Japan. The test results will allow the estimation of uncertainty measures associated with wind tunnel testing in various laboratories contributing to the database.

The talk will describe the methodology employed in the estimation of wind effects by the database-assisted design technique. This includes an overview of WiLDE (Wind Load Design Environment), which is a promising program that estimates peak statistics pertaining to non-Gaussian random processes. Illustrations of results that employ those methodologies will be based on selected wind tunnel measurements.



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NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: María De Lourdes Santiago Soto	**Grant Number:** 70NANB4H1024
Academic Institution: Inter American University of Puerto Rico, San Germán Campus	**Major:** Chemistry
Academic Standing as of September '04: Senior	
Current Career Plans: Plan to go to graduate school to pursue studies in Analytical Chemistry.	
NIST Laboratory, Division and Group: Chemical Science & Technology Laboratory, Surface and Microanalysis Science Division, Analytical Microscopy Group	
NIST Research Advisor: Dr. Greg Gillen	
Title of Talk: Advanced Inkjet Printing Technology for Trace Explosive Standards	

Abstract of Talk:

After September 11, national security has become a high priority for the United States. Instruments, such as Ion Mobility Spectrometers (IMS), are used in vulnerable places to detect explosives on surfaces. NIST is working to develop standard test materials to ensure proper operation and to characterize detection limits of IMS instruments. To accomplish this, a team of nine people is working with a drop-on-demand inkjet printer to produce test standards that contain known amounts of explosives for use on IMS instruments. The inkjet printer produces drops by the application of a voltage pulse to a piezoelectric material that is coupled to the fluid. When a drop is desired, the voltage is applied, and drops are generated from a 50 μm orifice printhead. The solutions in the printhead contain RDX, TNT, or PETN at known concentrations. The printer is controlled by a program that can vary the drop volume or the number of drops per spot. Various geometrical designs including fingerprints and arrays can be printed that contain high explosive material and dye compounds.

The mass of explosive dispensed on a printed test standard is determined on the basis of solution concentration, drop volume, and number of drops. Gas Chromatography-Mass Spectrometry is being used to verify the amount of explosive dispensed under the conditions used to prepare the test standards. The volume of the average drop is being determined by several techniques, including using a digital camera to image the drops under a high frequency strobe illumination, jetting the drops onto a non-wettable surface, and direct weighing of a large number of drops dispensed into a container.

The prepared test standards will be characterized by checking the IMS instrument response. A successful completion of this project leads the way to a rapid and reproducible method of preparing reference materials for the thousands of IMS instruments deployed at US airports.

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NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Karolina A. Sarnowska | **Grant Number:** 70NANB4H1040

Academic Institution: Mississippi State University | **Major:** Computer Science and Mathematics

Academic Standing as of September '04: Senior

Current Career Plans: Plan to go to graduate school to pursue studies in computer science and mathematics.

NIST Laboratory, Division and Group: Information Technology Laboratory, Advanced Network Technology Division, High Speed Networking Group

NIST Research Advisor: Dr. David Griffith

Title of Talk: A Comparison of Contention Resolution Schemes for Optical Burst Switching Networks

Abstract of Talk:

Optical Burst Switching (OBS) is a data transport architecture for optical networks that allows users to transmit information in large chunks known as bursts without reserving network resources for the duration of the connection. This approach allows multiple users to share network resources thus using bandwidth more efficiently.

Data that crosses an OBS network remains in optical form and is never turned into an electrical signal. This means that the data cannot be buffered in memory for an arbitrary period of time the way that packets can be in the conventional Internet. This causes a problem in OBS switches when bursts from different input ports attempt to use a single output port at the same time; only one burst can be transmitted while the other contending bursts are lost. This leads to relatively high burst loss rates that reduce the efficiency of the network by forcing retransmission of lost data. The research community has expended considerable effort over the last few years developing techniques to resolve contentions at output ports. Three techniques that have received the most attention are wavelength conversion, deflection routing, and fiber delay lines. These approaches can be applied to decrease the burst loss rate and allow greater utilization of the wavelengths in the network.

To date, there have been no examinations of the effect of using various combinations of these schemes. In order to provide design guidelines for future OBS networks, we conducted a comparative study of all the possible combinations of these techniques by applying existing theoretical models with extensions that we developed. Using these models we determined how much traffic each wavelength could support while maintaining an acceptably low burst loss rate. We used this information to conduct simulations in Matlab of a continental wide area network (WAN) using OBS with these contention resolution schemes. Our results show that it is possible to achieve very high wavelength utilization when various combinations of these techniques are used, giving very high performance gain with respect to circuit switched networks. We have laid the groundwork with this project to study the benefits of other contention resolution schemes in future research.

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August 10 – 12, 2004

Name: Andrew Schwarzkopf	**Grant Number:** 70NANB4H1013
Academic Institution: Cornell University	**Major:** Physics
Academic Standing as of September '04: Junior	
Current Career Plans: Graduate school, potentially for physics or biophysics	
NIST Laboratory, Division and Group: Physics Laboratory, Atomic Physics Division, Quantum Processes Group	
NIST Research Advisor: Dr. Garnett Bryant	
Title of Talk: Size-Dependent Optical Properties of Gold Nanotubes	

Abstract of Talk:

The optical properties of nanorods and nanorings have been used to enhance spectroscopy, to the extent of enabling single-molecule Raman spectroscopy. This is accomplished by magnifying the local electric field strength around the molecule, which can be done by a factor of roughly three hundred with a coupled-nanorod system.

To understand this field enhancement, we calculate far fields and near fields of Au nanorods by solving Maxwell's equations. However, previous calculations of the nanorods' effect on the light have used dielectric constants measured for bulk Au, not Au structures as small as the nanorods. A material's dielectric constant is actually size-dependent, classically seen to be a result of damping effects from electrons interacting with the surface. There was some fear that the damping effect would reduce the electric field enhancement of the system.

A quantum mechanical theory of size-dependent dielectric constants was applied to this problem, and the new results were compared with previous bulk-dielectric results. Results from various sizes and configurations of the nanorods were compared to see where non-bulk effects become more important.

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NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Eric Shamay	**Grant Number:** 70NANB4H1068
Academic Institution: California Polytechnic State University	**Major:** Chemistry, Engineering
Academic Standing as of September '04: Graduated	
Current Career Plans: Plan to go to graduate school to pursue studies in analytical chemistry.	
NIST Laboratory, Division and Group: Chemical Science and Technology, Chemical Properties Division, Experimental Kinetics and Thermodynamics Group	
NIST Research Advisor: Dr. Donald Burgess	
Title of Talk: Accessing Modern Real Fuels: Kinetic and Thermodynamic Property Databases	

Abstract of Talk:

Today's combustion research community suffers from a lack of centralized data on thermochemical and kinetic combustion properties. Current unevaluated databases only serve as compilations of data and do not hold any particular use for researchers seeking "best values", while critically evaluated databases are not current and are updated infrequently. A strong need has been identified for a compilation of complete reduced chemical kinetic models, and an accessible interface with tools and translators to allow researchers to compare the data.

Work has begun to create a centralized chemical kinetic database for real fuels. The database has been designed to contain thermochemical property data ($\Delta_r H°$, $S°$, $C_p°$, etc.) for fuel components and reaction intermediates, elementary rate coefficients (k) of combustion reactions, and chemical kinetic models for combustion simulations. A web-based interface prototype was created to access and introduce cross-referencing of the data to existing databases (NIST Chemical Kinetic Database and the NIST Chemistry WebBook). Various tools for data comparison, visualization, and translation have been employed.

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NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Brian J. Simonds	**Grant Number:** 70NANB4H1022
Academic Institution: Illinois Wesleyan University	**Major:** Physics
Academic Standing as of September '04: Senior	
Current Career Plans: Attend graduate school to pursue a PhD in physics.	
NIST Laboratory, Division and Group: Electronics and Electrical Engineering Laboratory, Quantum Electrical Metrology Division, Fundamental Electronic Measurements Group	
NIST Research Advisor: Neil Zimmerman, Manolis Hourdakis	
Title of Talk: Creating a Nanocapacitor to Measure the Energetics of Molecules in Self-Assembled Monolayers	

Abstract of Talk:

We have created a parallel-plate nano-capacitor measuring 80 microns by 80 microns with spacings between 50 and 70 nanometers with a dielectric of vacuum. This is the equivalent of having two sheets of metal the sizes of football fields lying on top of each other and separated by only 5 centimeters of empty space. Preliminary tests show that we can consistently obtain capacitance readings that scale for this configuration. By introducing a self-assembled monolayer on one plate of the capacitor and reading a change in capacitance as a potential difference is increased across the plates, we can relate the Fermi energy of the metal plate to the HOMO-LUMO gap energies of the molecules. We will characterize the gap energies of those molecules being pursued for use in molecular electronics and computing.

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NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Alan M. Skaggs	**Grant Number:** 70NANB4H1014
Academic Institution: Southern Methodist	**Major:** Mechanical Engineering & Math
Academic Standing as of September '04: Senior	
Current Career Plans: Plan to go to graduate school to pursue studies in mechanical engineering	
NIST Laboratory, Division and Group: Manufacturing Engineering Laboratory, Manufacturing Metrology Division, Manufacturing Process Metrology Group	
NIST Research Advisor: Dr. Robert W. Ivester	
Title of Talk: Cutting Forces in Aluminum Alloys	

Abstract of Talk:

Manufacturing processes are inherently complex; as a result, process development is often ad hoc and empirical. Process parameters, such as machining speeds, feed rates, and tool selection, are typically chosen by costly, trial-and-error prototyping, with the result that solutions are often sub-optimal. These sub-optimal practices are estimated to cost U.S. industry $10 billion per year. Pressure from international competitors is driving U.S. industry to seek more sophisticated and cost-effective means of choosing process parameters through modeling and simulation.

A principal barrier to reducing inefficiencies is the lack of access to validated, physics-based models of the manufacturing processes when key engineering decisions are made. Although there has been significant progress in the predictive simulation of low-strain-rate manufacturing processes such as forming, rolling, and drawing, there is a need for better predictive capabilities for high-strain-rate processes such as machining. The state of the art in predictive modeling of machining operations is severely limited because measurement and materials characterization capabilities are lagging model development. In other words, current models give impressive qualitative results, but there are virtually no data with which to validate these results.

Towards this end, machining temperatures and forces for orthogonal cutting of aluminum (AL7075-T651) were measured using dual-spectrum, high-speed video and 3-axis force measurement. These recorded values will then be used to benchmark model-based predictions of these and other machining measurements to establish baseline capabilities for predictive science-based modeling.

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August 10 – 12, 2004

Name: Kellie M. Smith	**Grant Number:** 70NANB4H1040
Academic Institution: Mississippi State University	**Major:** Chemical Engineering
Academic Standing as of September '04: Senior	
Current Career Plans: Plan to begin graduate school in August 2005	
NIST Laboratory, Division and Group: Chemical Science and Technology Laboratory, Analytical Chemistry Division, Organic Analytical Methods Group	
NIST Research Advisor: Dr. Bryant C. Nelson and Dr. Mary B. Satterfield	
Title of Talk: Determination of Folate Vitamers in Spinach via Liquid Chromatography Combined with Ultraviolet and Fluorescence Detection	

Abstract of Talk:

Folates are a complex group of water-soluble B vitamin isoforms (vitamers) whose most recognized isoform is a compound called folic acid (FA). Deficiency of folates in the diet is linked to increased risk of neural tube birth defects in newborns and to increased risk of cardiovascular disease in adults. Folate vitamers in food matrices are commonly found covalently conjugated to multiple (2 - 7) glutamic acid residues (polyglutamates). 5-Methyltetrahydrofolic acid (5MT) and 5-formyltetrahydrofolic acid (5FT) are two of the most abundant folate polyglutamates found in fresh spinach. The research contained in this presentation describes the preliminary development of an analytical method to determine the folate levels in NIST spinach SRM 2385. To more accurately determine the level of each folate vitamer present in spinach, folate conjugase (a hydrolytic enzyme) can be used to convert the heterogeneous polyglutamate folate forms to a single monoglutamate form. High performance liquid chromatography, specifically reversed phase liquid chromatography, coupled with fluorescence detection and ultraviolet detection was used to separate and quantitatively detect the relevant folate forms. Preliminary folate deconjugation experiments were performed using commercially available folic acid triglutamate (FA-3Glu). Rat plasma conjugase was used to convert FA-3Glu to folic acid monoglutamate (FA-1Glu). Analytical conditions required for optimal conversion of FA-3Glu to FA-1Glu were developed. Finally, the sensitive detection of FA-1Glu was enhanced through the use of off-line solid phase affinity extraction clean-up procedures. These optimized procedures can now be extended to the quantitative determination of 5MT and 5FT polyglutamates in spinach.

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NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Paul Speicher

Grant Number: 70NANB4H1059

Academic Institution: University of Virginia

Major: Physics & Biology

Academic Standing as of September '04: 3rd year

Current Career Plans: Plan to attend medical school; pursue career as a surgeon

NIST Laboratory, Division and Group: Physics Laboratory, Ionizing Radiation Division, Radiation Interactions and Dosimetry Group

NIST Research Advisor: Dr. Heather Chen-Mayer

Title of Talk: Ionizing Radiation Dosimetry Using Water Calorimetry: The Exciting World of Water Temperature

Abstract of Talk:

Radiation dosimetry for applications in all areas including radiation protection and radiation therapies needs to be traceable to a primary standard maintained at NIST. The primary standard for air-kerma (kinetic energy transferred per unit mass - in air) is currently based on graphite cavity ionization chambers. A much more direct approach to clinical radiotherapy calibration is done based on the concept of absorbed dose, that is, the amount of ionizing radiation actually absorbed by living tissue, or more practically, water, which displays nearly identical response characteristics. The current primary standard for absorbed dose to water was established in the early 90's using a water calorimeter that is no longer operational. Our group has been working with a second generation water calorimeter to both verify existing standards and to re-establish a working primary dosimetry standard. Using a modified Wheatstone bridge equipped with thermistors to measure water temperature rise due to incident gamma radiation from a Co-60 source, both the traditional time-domain and the newly developed frequency-domain analyses have yielded mutually consistent results. However, the new result is 6-7% lower than the transferred historical value. Investigation of the impacts of circuit capacitance, changing thermistor characteristics, and environmental temperature variations on the accuracy of our time-domain analysis routine has revealed some very interesting phenomena. Through our progression in understanding and interpreting this behavior we have moved closer to the realization of a primary standard of absorbed dose to water.

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August 10 – 12, 2004

Name: Christopher J. Stanford	**Grant Number:** 70NANB4H1011
Academic Institution: University of Southern California	**Major:** Physics
Academic Standing as of September '04: Senior	
Current Career Plans: Attend a graduate program in electrical engineering to study photonics.	
NIST Laboratory, Division and Group: Physics Laboratory, Atomic Physics Division, Plasma Science Group	
NIST Research Advisor: Dr. Erick Benck	
Title of Talk: Sub-millimeter Absorption Spectroscopy of Water Vapor	

Abstract of Talk:

As IC device dimensions continue to shrink the semiconductor industry requires increasingly precise plasma etching of device features. Achieving such refined control of the etch process requires sensitive diagnostics for process characterization. Sub-millimeter spectroscopy is a new method of characterizing plasma chamber conditions that is capable of sensitive measurements of plasma species concentration, of the order of 1 ppb. In this work, initial exploration of the detection limits of this novel spectroscopy was performed by measuring trace water vapor contamination of nitrogen. The broadband millimeter wave source used was a recently developed planar diode multiplier chain, which covers the range 525-625 GHz. Output was detected by a cryogenically cooled InSb hot electron bolometer. The sub-millimeter source was frequency scanned across the strong 556935.9 MHz water absorption line and detection was done using two methods. Simple absorption detection (AM) was first used for absolute measurement of water vapor concentration. Further measurements were made using 2nd harmonic frequency modulation (FM) detection, which is capable of detecting weaker signals expected from trace gases. Results of this ongoing work are presented.

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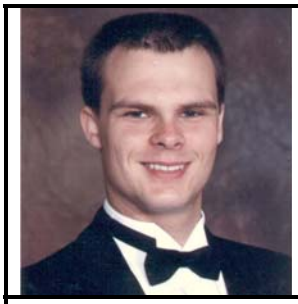
NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Anna Stelzenmuller	**Grant Number:** 70NANB4H1014
Academic Institution: Southern Methodist University	**Major:** Electrical Engineering and Physics
Academic Standing as of September '04: Senior	
Current Career Plans: Continue to Graduate School in Electrical Engineering	
NIST Laboratory, Division and Group: Electronics and Electrical Engineering Laboratory, Semiconductor Electronics Division, Microelectromechanical Systems Group	
NIST Research Advisor: Dr. Brian J. Polk	
Title of Talk: Surface Treatment and Characterization of Ag/AgCl Micro-Reference Electrode Arrays for BioElectronics	

Abstract of Talk:

Reference electrodes are necessary for the meaningful measurement of potentials in biological and chemical experiments with wide applications in healthcare, biotech and other industries. Currently, the Ag/AgCl electrode serves as a popular reference in laboratories. However, with its "dip-stick" configuration, these electrodes are too cumbersome for many micro-applications, particularly those involving microfluidic channels. To address the need for a standard, miniaturized reference, an array of Ag/AgCl microelectrodes was designed, fabricated and characterized. Fabrication of these devices involved photolithographic techniques on silicon substrates followed by electrochemical surface treatments. Open circuit potential measurements examined the stability of the microelectrodes over time, and impedance experiments described the interfacial chemical processes. Characterizations of the microelectrodes in bulk solutions allowed for comparison against commercially available Ag/AgCl reference electrodes, demonstrating an agreement within +/-2mV. Additional testing of the microelectrodes in microfluidic channels monitored their behavior under smaller volume conditions with microchannel dynamics. Offering a stable reference potential and the possibility of integration with electronic circuits, these Ag/AgCl micro reference electrode arrays will benefit bioelectronics research and industry efforts towards single cell characterization.



SURF Student Colloquium

NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Tracy Stover	**Grant Number:** 70NANB4H1063
Academic Institution: Murray State University	**Major:** Engineering Physics
Academic Standing as of September '04: Senior	
Current Career Plans: Plan to go to graduate school for nuclear engineering.	
NIST Laboratory, Division and Group: Chemical Science & Technology Laboratory, Center for Neutron Research, Analytical Chemistry Division (839), Nuclear Methods Group	
NIST Research Advisor: Dr. George Lamaze	
Title of Talk: Compton Suppression for Neutron Activation Analysis Applications at the National Institute of Standards and Technology	

Abstract of Talk:

Suppression systems reduce Compton backscattering counts in a spectrum. This study examines three Compton suppression systems at the NIST Center for Neutron Research in an effort to produce a general guide to their setup and use rather than specific settings for a certain experiment, since every system has particular calibration nuances due to differences in electronics, detectors, and environment. Also presented are several troubleshooting procedures for timing and calibration of these systems.

A central HPGe detector is surrounded by guard detectors. Counts picked up by both detectors are Compton or escape events, while those detected only by the HPGe are photopeaks considered useful for analysis. The electronics system is designed to record counts detected only by the HPGe detector and reject ones in coincidence with the guard detectors. To show the suppression effect, calibration sources Cs-137, Na-24, and Co-60 were analyzed. Certified reference materials, activated in the reactor, were examined to demonstrate experimental readiness of the systems.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Stephanie Svetlik	**Grant Number:** 70NANB4H1044
Academic Institutions: Pomona College	**Major:** Physics
Academic Standing as of September '04: Masters student	
Current Career Plans: Attending graduate school in pursuit of a doctorate in structural materials	
NIST Laboratory, Division and Group: Building and Fire Research Laboratory, Materials and Construction Research Division, Polymeric Materials Group	
NIST Research Advisors: Dr. Stephanie Scierka and Dr. Peter Votruba-Drzal	
Title of Talk: Nanomechanical Properties of TiO_2/Epoxy Nanocomposites	

Abstract of Talk:

Inorganic fillers, such as Titanium Dioxide (TiO_2), have historically been added to polymeric coatings to enhance the appearance properties and mechanical durability of coatings. It is known that polymeric films containing TiO_2 exhibit measurable photocatalytic degradation after exposure to ultraviolet (UV) irradiation. A highly reactive TiO_2 particle system with a particle size of 25 nm and a coated, less reactive TiO_2 particle system with a particle size of 250 nm were incorporated into a model epoxy system with a pigment volume concentration (PVC) of 10%. The films were exposed to UV irradiation using Simulated Photodegradation by High Energy Radiant Exposure (SPHERE). Degradation from UV exposure was examined using Attenuated Total Reflectance (ATR) Fourier transform Infrared Spectroscopy (FTIR). The effects of degradation and particle size on mechanical properties were measured on both the bulk and nano scale by performing dynamic material analysis (DMA) and nanoindentation.

SURF Student Colloquium

NIST – Gaithersburg, MD

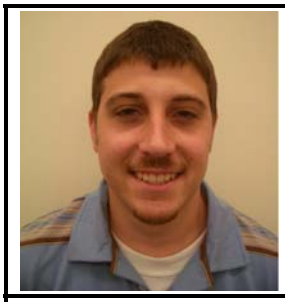
August 10 – 12, 2004

Name: Wei M. Tan	**Grant Number:** 70NANB4H1023
Academic Institution: University of Colorado	**Major:** Electrical Engineering
Academic Standing as of September '04: Senior	
Current Career Plans: Plan to go to graduate school to pursue studies in electrical engineering.	
NIST Laboratory, Division and Group: Electronics and Electrical Engineering Laboratory, Semiconductor Electronics Division , Enabling Devices ICs Group	
NIST Research Advisor: Dr. Michael Cresswell	
Title of Talk: Investigation of Carbon Contamination of CD Reference Materials	

Abstract of Talk:

This SURF project is to investigate the prospects using Scanning Electron Microscopy (SEM) as a transfer metrology for critical dimension (CD) reference features and to assess the amount of apparent CD growth caused by carbon contamination during SEM imaging.. This work builds on an on-going EEEL project to provide CD reference features to the semiconductor industry. Other directions have included using electrical CD (ECD) metrology and atomic force microscopy (AFM) as the transfer metrology. In all of these techniques, the primary calibration is via High Resolution Transmission Electron Microscopy (HRTEM). A transfer method is required when using HRTEM because HRTEM destroys the features.

To investigate a SEM-based transfer metrology, images were acquired from a number of reference features on multiple chips, and the CD of each feature was measured one or more times. The features that were measured repeatedly were selected to detect drift in the SEM and/or physical changes to the feature caused by of the deposition of carbon contamination by the electron beam. The raw image data from the SEM was then analyzed using commercial tools, in this case, CorelDRAW and Image-Pro. The analysis based on the features measured twelve times shows an expected apparent "growth" of the CD as the samples accumulated contamination as a function of the total time that they were exposed to the electron beam. The growth rate was approximately 2 nm per image. A factor two higher growth rate was observed for the features at the borders of the images. As a result of this study, this is likely due to the beam scanning dynamics, potentially a useful discovery for nanotechnology. In this experiment we see that the SEM can be used for transfer metrology, but although we expect it to lead to a combined uncertainty better than that observed when using ECD as the transfer metrology, it will be worse than when using AFM as the transfer metrology.



SURF Student Colloquium

NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Alan A. Thrift	**Grant Number:** 70NANB4H1037
Academic Institution: Univ NC at Charlotte	**Major:** Mechanical Engineering
Academic Standing as of September '04: Senior	
Current Career Plans: Plan to go to graduate school to pursue studies in Mechanical Engineering.	
NIST Laboratory, Division and Group: Material Science and Engineering Laboratory, Center for Neutron Research, Neutron Condensed Matter Science	
NIST Research Advisor: Dr. Thomas Gnaupel-Herold	
Title of Talk: Mechanical Design of a Uniaxial Load Frame with High Load Capacity	

Abstract of Talk:

Dr. Thomas Gnäupel-Herold's research focuses on residual stresses in materials using neutron diffraction. Residual stresses occur as the result of inhomogeneous distortions in almost all materials. These distortions are caused by mechanical, thermal or chemical treatments that affect a specimen (the 'part') inhomogenously, e.g. only at the surface. They can be measured using diffraction by probing the distance between lattice planes in crystalline materials. By comparing the lattice distortions with a reference value, e.g. from an unstressed specimen, lattice strains can be obtained which, in turn, translate into stresses by means of Hooke's law. The unique advantage of neutron diffraction is their penetration, which, for most materials is of the order of centimeters. This property allows the non-destructive evaluation of 3D stress fields in industrial components such as rails or car parts. However, there is also a strong interest in utilizing this technique for investigating basic phenomena of plastic deformation in materials on the scale of the crystalline constituents. This can be done by applying a stress to a material while scanning the resulting 3D distortions in a single grain. This basically means scanning through several locations of a single grain using a neutron beam of about 1-mm in size (limited by neutron flux). In order to obtain sufficiently detailed distortion/stress maps the grain size should be several millimeters, which requires a specimen cross section greater than 1 cm^2. The forces required to deform such a specimen are of the order of 10 tons. However the load frame currently being used is only capable of producing approximately 1 ton of force. The current load frame is also very small so sample size is extremely limited and the space around the sample is cluttered making access to the sample quite difficult. Therefore I was asked to design and construct a uniaxial load frame with a much higher load and sample capacity. Over the course of the summer I was successful in designing a load frame that is capable of producing forces up to 15 ton tensile or compressive loads and supporting a maximum sample size of 8 inches with fifty-percent strain. The newly designed load frame can still fit on the same experiment table as the old load frame and be rotated about 360 degrees on the experiment table without hitting any of the surrounding equipment. The space around the sample is open on all sides making the sample accessible by the neutron beam and the measuring apparatus. The load frame incorporates a simple control system that utilizes a feedback loop between the load cell and stepper motor. The user simply indicates what load is desired on the sample and the stepper motor drives until the load cell reads the corresponding load. The size of the load frame is sufficient to incorporate ancillary equipment such as a second, smaller load frame for biaxial loads, or sample heating devices. Finally the load frame is completely transformable. It can be made larger or smaller depending on the sample or experiment table setup size. Dr. Gnäupel-Herold will be using the new and improved load frame to extend his research on residual stresses and deformation of materials.

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NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Felicia Tsai

Grant Number: 70NANB4H1034

Academic Institution: Rensselaer Polytechnic Institute

Major: Chemistry

Academic Standing as of September '04: Junior

Current Career Plans: To pursue higher education in the field of chemistry and conduct research at a scientific institution

NIST Laboratory, Division and Group: Chemical Science and Technology Laboratory, Surface and Microanalysis Division, Analytical Microscopy Group

NIST Research Advisors: Dr. Greg Gillen and Dr. Christine Mahoney

Title of Talk: Analysis of a Model Drug Delivery System Using Cluster Secondary Ion Mass Spectrometry (SIMS) and Trace Narcotics Detection Using Ion Mobility Spectrometry (IMS)

Abstract of Talk:

Two methods of trace drug and narcotic detection are explored. Time-of-Flight Secondary Ion Mass Spectrometry (TOF-SIMS) is a promising technique for the analysis of drug delivery systems. With SIMS we have the capability to monitor the distribution of both drugs and excipients in drug delivery systems both spatially and in some cases as a function of depth when using a polyatomic primary ion source (such as SF_5^+). Here we utilize cluster SIMS depth profiling to monitor the distribution of a model drug (4-acetamidophenol) in a poly(lactic acid) (PLA) matrix. We were able to successfully monitor the distribution as a function of depth for concentrations of 0, 2, 5, 7, 10, 15, and 20 percent (w/w) 4-acetamindophenol. From this data, calibration curves were created which were the bases for quantification. The intensity variations within the profile indicated that there was a drug depleted surface region. Affirmation of this depletion layer was evident by the consistency between the intensity variations of the isotopic labeled drug fragment ions and the drug molecular ion. Ion Mobility Spectrometry (IMS) is an effective tool in trace explosives detection and is highly utilized for homeland security applications. However, it is also potentially useful for narcotics detection. Its capacity for narcotics detection was investigated. Standard solutions of 9 different illicit narcotics were prepared, and the IMS performance was characterized. A study on detection limits showed variability dependent on each drug. It was found that amphetamines, MDA, MDMA, morphine, and heroin had a lower limit at ~25 ng. Cocaine, methamphetamines, and flunitrazepam had yet a lower limit at ~6 ng.

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August 10 – 12, 2004

Name: Angel L. Villalain-Garcia	**Grant Number:** 70NANB4H1046
Academic Institution: University of Puerto Rico	**Major:** Computer Engineering
Academic Standing as of September '04: Fourth year of a five year program	
Current Career Plans: Plan to go to graduate school to pursue studies in computer science.	
NIST Laboratory, Division and Group: Information Technology Laboratory, Mathematical and Computational Sciences Division, Scientific Applications and Visualization Group	
NIST Research Advisor: William George	
Title of Talk: Authentication and Authorization in a Distributed Computer Server	

Abstract of Talk:

This project adds security measures, including authentication and authorization, to Screen Saver Science (SSS), a project to create a general distributed computing environment. The need for computing resources is growing each day. This need has inspired many innovative advances, such as the use of clusters to meet the computational need. However, in some situations, acquiring and maintaining a cluster may be too expensive. Another solution that has emerged recently is to harness the computing resources that are already connected by a network to create a dynamic distributed computing system. This scheme can increase the available computing power, without additional hardware, by taking advantage of temporarily unused, or under-used, computer on the network. This is the basic approach of the NIST SSS Project. There are other applications, such SETI@Home, Folding@Home and others, that follow this same basic approach, but these other examples differ from SSS in important ways. Most importantly, SSS provides a general purpose computing platform in which programs can be submitted for execution at any time, by any of the participants, without requiring the clients, which perform the computations (task), to pre-install files or pre-configure their machines in any way. The SSS clients can specify preferences for tasks form certain people or projects, but all SSS clients are eligible to run any available tasks that their machines are capable of running. A priority system helps prevent tasks from forever being ignored and also helps high priority tasks to be executed promptly.

SSS attempts to deal directly with security concerns. The SSS clients, which form the computer resource in SSS, obtain the SSS service by locating and downloading code each time it runs. For security reasons, the client must ensure that the code is trusted, preventing imposters and malicious code from being executed by the SSS clients. Once trusted, the SSS client can then authorize the code to use local resources and to execute the code it needs to complete its tasks. Similarly, the SSS service ensures that only valid SSS clients run the SSS tasks. The security aspects in SSS are provided by JINI and are based on standard Java packages such as the Java Authentication and Authorization Service (JAAS), and the Java Cryptographic Extension (JCE).

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August 10 – 12, 2004

Name: David C. Walker	**Grant Number:** 70NANB4H1030
Academic Institution: University of Rochester	**Major:** Computer Science
Academic Standing as of September '04: Senior	
Current Career Plans: Complete undergraduate studies and possibly pursue a Ph.D. in computer science	
NIST Laboratory, Division and Group: Manufacturing Engineering Laboratory, Manufacturing Systems Integration Division, Manufacturing & Modeling Simulation Group	
NIST Research Advisor: Frank Riddick and Chuck McLean	
Title of Talk: A Standard Architecture for Naval Training Simulations	

Abstract of Talk:

In the motion picture and gaming industries, a variety of multimedia techniques are used to enhance the realism and fidelity of the end product. Such techniques are also useful for creating realistic simulations that can be used for purposes other than entertainment, such as training. NIST has been working with the Navy Education & Training Command in order to develop a standard architecture for training simulations based on motion picture and video game technologies. By developing such an architecture, and from it a standard simulation engine, the Navy hopes to save on development and deployment costs for future training simulations.

Of particular importance to realistic simulations is physics-based motion. For relatively simple simulations, a physics engine should support rigid-body dynamics, basic joint constraints, collision detection, and collision response. As simulations become more complex, it becomes necessary to incorporate reasonably accurate physics for soft-body dynamics, more complex joint constraints, sophisticated collision detection and response, and fluid dynamics.

The talk will cover the research and development work done on the architecture and the engine during the summer of 2004. Included in the discussion will be topics such as problems encountered during development and the factors driving our decisions on components to use. The talk will also feature demonstrations of the engine in its preliminary stages, with particular focus on the physics and graphical aspects.

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NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: MacArthur Weatherspoon II	**Grant Number:** 70NANB4H1004
Academic Institution: University of Cincinnati	**Major:** Nuclear Engineering
Academic Standing as of September '04: First year grad student	
Current Career Plans: Plan to go to graduate school to pursue studies in nuclear engineering.	
NIST Laboratory, Division and Group: Physics Laboratory, Ionizing Radiation Division, Neutron Interactions & Dosimetry Group	
NIST Research Advisor: Dr. David Gilliam	
Title of Talk: Neutron Spectroscopy	

Abstract of Talk:

One of the objectives in the Neutron Interactions and Dosimetry group is to find more effective neutron detection methods for the task of improving homeland security within our Nation's transportation system for goods and other commerce. Conventional methods of detection are proving insufficient for the increasing threat of nuclear weapons and radioactive substances stored in large shipping containers. As a result, the role of radioactive sensors and detection equipment designed to inspect large traffic areas has greatly increased in the last few years. Knowing that it takes one to know one, a good detection instrument for radioactive material in large containers is a neutron spectrometer. Neutron detectors have much lower background count rates than gamma-ray detectors. I am running Monte Carlo simulations of neutron spectrometer designs, and developing an auxiliary program in C++ for interpretation of the Monte Carlo results. Our goal is the development of a highly efficient, compact neutron spectrometer with good energy resolution and very low response to natural background radiations.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: James E. Wells	**Grant Number:** 70NANB4H1056
Academic Institution: Davidson College	**Major:** Physics
Academic Standing as of September '04: Sophomore	
Current Career Plans: Continuing the study of physics into graduate school	
NIST Laboratory, Division and Group: Building and Fire Research Laboratory, Materials and Construction Research Division, Polymeric Materials	
NIST Research Advisor: Dr. Christopher White and Dr. Emmett O'Brien	
Title of Talk: The Design and Fabrication of a Thermally Driven Outdoor Sealant Tester	

Abstract of Talk:

Building joint sealant (caulk) is a vital, yet understudied component in the construction of buildings. Often chosen for low cost rather than high quality, the failure of building sealants is a major contributor to the almost $75 billion Americans spend on home repairs each year. One cause of this is that current sealant testing methods are neither precise nor accurate, nor do they lead to predictions about the causes of sealant failure. In addition they are both costly and time consuming. As part of a larger effort to develop new and better testing methods for building sealant, a second-generation thermally driven outdoor sealant tester was constructed.

The outdoor sealant tester is held in place by a static wood and stainless steal frame, and driven by the thermal expansion of PVC (Polyvinyl Chloride) pipes. The expansion and contraction of the pipes causes the sealant samples to undergo compression and expansion. Two Linear Variable Differential Transformers and a miniature load cell record these events. This data can be analyzed to determine the stress-strain information for the samples, which can then be correlated with environmental data such as temperature or solar flux. The data gathered from the outdoor sealant tester will be compared to NIST/BFRL laboratory predictions.

As part of a separate experiment, an outdoor exposure apparatus was constructed to determine the relationship between solar radiation and the temperature of light and dark colored steel tiles with thin polymeric coatings. The data collected from this apparatus will be used to evaluate a mathematical temperature model, which will serve as a tool to predict the durability of these types of coatings in the outdoor environment.

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NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Kevin A. Wepasnick	**Grant Number:** 70NANB4H69
Academic Institution: Franklin & Marshall College	**Major:** Chemistry
Academic Standing as of September '04: Junior	
Current Career Plans: Plan to go to graduate school to pursue studies in chemistry.	
NIST Laboratory, Division and Group: Chemical Science and Technology Laboratory, Physical and Chemical Properties Division, Computational Chemistry Group	
NIST Research Advisor: Dr. Thomas C. Allison	
Title of Talk: Web-based Databases for Chemical Properties	

Abstract of Talk:

NIST has a long history of high-quality data publications. In recent years, an increasing amount of NIST data has been disseminated via the web, which makes it readily accessible to a large number of data consumers. This talk will focus on efforts to create web interfaces for two NIST projects.

The first of these projects is a collection of data on aromatic species from a variety of sources. Drawing on material for NIST Special Publications 922 and 928 as well as semiemperical molecular orbital calculations, a useful collection of data on aromatic compounds was created. The web interface allows simple access to all of the data via searching and browsing. The types of data present range from fundamental thermodynamic data to Henry's Law Constants.

In the second project and interface for collecting and disseminating data on atomic and molecular clusters was created. This interface will allow NIST scientists to share their experimental and theoretical data on aromatic clusters with the scientific community. It will further allow NIST to collect similar data from the community. With this data in hand it will be possible to deeply investigate the mechanisms whereby atoms and molecules aggregate to form nanoparticles.

In any data project concerned with putting data on the web it is important to use the right tools and programming practices. In these projects we have sought to use the best-of-breed Java tools such as Java Server Pages (JSP). The infrastructure supporting the web interface relies on open-source software such as Jakarta Tomcat, mySQL, and Apache.

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NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Jennifer L. Wiley	**Grant Number:** 70NANB4H1049
Academic Institution: University of Maryland College Park	**Major:** Fire Protection Engineering
Academic Standing as of September '04: Junior	
Current Career Plans: Plan to go to graduate school to pursue studies in fire protection engineering.	
NIST Laboratory, Division and Group: Building and Fire Research Laboratory, Fire Research Division, Analysis and Prediction Group	
NIST Research Advisor: Dr. Kevin McGrattan	
Title of Talk: Validation Experiments for the Fire Dynamics Simulator, Version 4.0	

Abstract of Talk:

The Fire Dynamics Simulator (FDS) developed at NIST is a tool often used by practicing fire protection engineers and fire researchers. FDS is a computational fluid dynamics (CFD) model of fire-driven flows. In analyzing the output of FDS, users must be aware of the degree of reliability that can be expected from the program, as well as its strengths and weaknesses. This is especially important when a new version is introduced, as various aspects of the program have undoubtedly been changed. For this reason, validation experiments were conducted at NIST in order to evaluate the ability of the newest version of FDS, Version 4.0, to predict various aspects of smoke and fire spread. To do this, several full-scale fire tests were reconstructed in FDS. Because full-scale fire experiments are less controlled than bench scale experiments, each full-scale test was performed twice to determine the reproducibility of the test itself. Thermocouple data taken during the actual tests was compared to temperature data generated by FDS in order to assess the accuracy of the model. In addition, pictures and video taken of these tests were compared to visualizations produced by Smokeview, the companion program to FDS. Various parameters were adjusted in order to yield the room configuration and material properties that produced the best match to the thermocouple and visual data.

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NIST – Gaithersburg, MD

August 10 – 12, 2004

Name: Ramsey Zeitoun	**Grant Number:** 70NANB4H1049
Academic Institution: University of Maryland, College Park	**Major:** Chemical Engineering
Academic Standing as of September '04: Junior	
Current Career Plans: To get my graduate degrees in chemical engineering	
NIST Laboratory, Division and Group: Materials Science & Engineering Laboratory, Center for Neutron Research, Neutron Condensed Matter Science Group	
NIST Research Advisor: Dr. Terry Udovic	
Title of Talk: Development of a Bismuth Filter for the Filter Analyzer Neutron Spectrometer	

Abstract of Talk:

The neutron is a novel and powerful probe of condensed matter. It possesses no charge and interacts with atoms via nuclear rather than electrical forces, thus allowing it to penetrate through most materials. The wavelike properties of the neutron permits one to utilize diffraction methods to create beams of monoenergetic neutrons for use in such scattering techniques as neutron vibrational spectroscopy (NVS). NVS is analogous to photon-based vibrational spectroscopies such as infrared or Raman spectroscopy, but possesses unique properties that render it complementary to these spectroscopies and invaluable for probing the vibrational spectra of solid-state materials. One limitation of the Filter-Analyzer Neutron Spectrometer (FANS), the world-class NVS instrument at the NIST Center for Neutron Research (NCNR), is the presence of spurious low-level background scattering from the beryllium (Be) filter used in the scattered-neutron analyzer. Such spurious scattering complicates the clean measurement of the vibrational density of states of more weakly scattering samples. Here, it is determined that these spurious scattering can be eliminated by an additional "polycrystalline" bismuth (Bi) filter placed in front of the Be filter. The development of a Bi filter with sufficient polycrystallinity is nontrivial since bismuth tends to form unacceptably large crystallites upon solidification from the melt. To substantiate this discovery, diverse bismuth samples were studied using the SANS (Small Angle Neutron Scattering) instrument, and DCS (Disk Chopper Spectrometer) in order to characterize the neutron transmission of the samples. Metallurgical studies were also extensively sought after for characterization and information into ways to most appropriately optimize neutron transmission. With a prototype of the filter in place, and plans for creating the final one underway, low scattering samples such as dodecacalcium 14-aluminum oxide were analyzed and studied without fear of spurious scattering and false readings.

2004

SURF STUDENTS

by Laboratory

Student	University	Talk Title	OU
Acevedo-Velez, Claribel	University of Puerto Rico, Mayaguez	Automation of the NIST Hydrometers Calibration Service	CSTL
Adler, Alexander U.	The Pennsylvania State University	Phase Equilibria Studies of Bi2O3-MN203-Nb205	MSEL
Anttonen, Jennifer	Carnegie Mellon University	Determining Plasma Temperatures with Spectroscopic Data	PL
Armstrong, Matthew A.	Davidson College	The Effect of Temperature on the Fluorescence of Phycoerythrin and Oligonucleotide-Labeled Fluorophores	CSTL
Ashford, Dahlia	Mississippi State University	The Influence of Chemical and Environmental Factors on Measurements of the Degree of Hydration of Cement Pastes	BFRL
Ashley, William			ITL
Austin, Whitney B.	Jackson State University	Tracker Calibration for Immersive Visualization in a Reconfigurable Automatic Virtual Environment	ITL
Ban, Han Yong	Pomona College	Lifetime Measurement of Erbium Transition $4f^{12}6s^2 \rightarrow 4f^{11}(^4I^o_{15/2})\ 5d_{5/2}\ 6s^2$	PL
Baum, Caitlin E.	University of Maryland, Baltimore County	Characterizing Polymer Nanocomposites During Processing	BFRL
Baumgold, Ben	Massachusetts Institute of Technology	Magnetic Refrigeration: Perfecting the Process	MSEL
Blanchard, Daniel S.	Millersville University	Computer-Aided Camera Placement Software for Facial Recognition	ITL
Bonds, Quenton	University of Alabama, Birmingham	The Study of Metal Work Functions by Measurements of Capacitance- voltage, Scanning Kelvin Probe Microscopy	EEEL
Breidenich, Jennifer L.	Smith College	Investigating Interactions Between Colloidal Material and Polycyclic Aromatic Hydrocarbons: Quantifying Sorption Characteristics	CSTL
Brewer, Samuel M.	Appalachian State University	Visible Imaging of Highly Charged Ion Clouds in the NIST EBIT	PL
Brooks, Charles	University of Maryland, College Park	The Observance and Removal of PSS Top Layer in Poly(3,4-ethylenedioxythiophene)-polystyrenesulfonic Acid (PEDOT-PSS) Conducting Thin Films	MSEL
Burley, Shauntia	Coppin State University	Creating 3D Visualizations for the NIST Digital Library of Mathematical Functions	ITL
Butler, Alina	Mississippi State University	Evaluation of Alpha Spectra Deconvolution: A Beam Piercing Through the Vail of Obscurity	PL
Bykowski, Mikolaj	Lehigh University	Evaluating the Fire Resistance of Structural Steel	MSEL
Chang, Daphne	Duke University	In Search of Higher Pu Sensitivity for TIMS	PL
Chereck, Andrew Q.	Illinois Wesleyan University	Controlling a Josephson Junction Array with LabView	EEEL
Clarke, Michelle N.	Johns Hopkins Univeristy	Characterization of the Microstructure and Properties of Fire Protective Materials	BFRL
Cleveland, Thomas E.	Tulane University	Using Neutron Imaging to Analyze the Internal Structure of Biological and Mechanical Objects	PL
Cogut, Daniel A.	College of William and Mary	Fusion of Biometric Algorithms	ITL
Colleton, April	Rochester Institute of Technology	Electropolymerization and Functionalization of Polymeric Material for DNA Sensing in Microfluidic Channels	CSTL
Comer, Jeffrey R.	University of Akron	Fractional Kinetics in Atomic Forece Microscope Assisted Oxidation of Zirconium Nitride	MEL
Conrad, Brad R.	Rochester Institute of Technology	Time Domain Dielectric Spectroscopy Analysis of the Amorphous Phase in Semicrystalline Polycarbonate	MSEL
Cordes, Brian G.	Worcester Polytechnic Institute	Developing a Graphical Tool to Determine the Estimation Capacity of an Experimental Design	ITL
Davidson, Matthew	Catholic University	Quantum Cellular Automata Architecture in an Optical Lattice	PL
Diez, Dustin	Rhodes College	Calibration of a Micro Force Sensor for the Characterization of Compliant Mechanism MEMS	MEL
Farrar-Foley, Brendan	The George Washington University	PDA Forensic Tools: Overview and Analysis	ITL
Fisher, Nathan T.	University of Maryland, College Park	Correlating HMDS (Hexamethyldisilazane) Modified Silica Substrate Surface Characteristics to Thin Film Morphology of Poly(3-hexylthiophene)	MSEL
Frederick, Amanda	Miami University	Use of a Laser Vibrometer for Measuring Spindle Error Motion	MEL

Student	University	Talk Title	OU
Fried, Alexander	University of Pennsylvania	Digital Image Plate Diagnostics for Use in Ultraviolet Spectroscopy	PL
Fuentes-Figueroa, Angel G.	University of Puerto Rico, Mayaguez	Testing Software Packages for Gamma-Ray Spectrometry Measurements Using Germanium Detectors	PL
Gao, Jingsi	Delaware State University	Wireless Enhancement for Storage Networking	ITL
Garber, Chris S.	Austin Peay State University	Forensic Ballistics: Checking the Performance of Integrated Ballistics Systems with the Standard Bullet and Casing Project	EEEL
Gewuerz, Lloyd W.	Binghamton University, SUNY	The Capabilities of FDS for Prediction of the Steady-State Burning of Small-Scale Materials	BFRL
Goldfarb, Stephanie E.	Cornell University	Factors Influencing the Determination of the Strain Energy Release Rate of an Adhesive Tape	BFRL
Goodrum, Jr., William J.	University of Virginia	Microfluidic Interfacial Tension Measurements: Getting the Most From Your Soaps	MSEL
Griggs, Cornelius	University of Maryland, College Park	Investigating Mechanical Properties of Thin Films via Nanoindentation	MSEL
Harris, Theodore Robert	University of North Carolina, Charlotte	Combinatorial Study of Nickel-Gold p-contacts for Blue InGaN Light Emitting Diodes Comparing Electron Beam and Pulsed Laser Deposition Techniques	MSEL
Hoebel, Stacey J.	University of Wisconsin, Madison	Temperature Gradient Focusing	CSTL
Huber, Michael	American University	Streamlining the Production of Viewpoints in VRML	ITL
Hughes, Nicholas R.	Southern Methodist Univeristy	Chaotic Mixing in Microfluidic Devices	MSEL
Hwang, Jesse W.	University of Maryland, College Park	Development of Calcium Phosphate-gelatin Composites	MSEL
Jacques, Teresa L.	Smith College	X-ray Reflectivity Study of the Formation of Alkane Films on OTS-coated Silicon Surfaces	MSEL
Jalilian, Firouzeh	University of Maryland, College Park	Developing a Graphical User Interface for the Mass Calibration Program	ITL
Jenkins, Dyami H.	University of Maryland, College Park	Augmentation of the Statistical Test Suite for Random Number Generators	ITL
Johnson, Soren	Boston University	An Intrusion Detection System in a Wireless Ad Hoc Network	ITL
Kelsic, Eric D.	California Institute of Technology	Efficient Implementation of Error-Handling for Quantum Key Distribution	PL
Kim, Meeri N.	Boston University	Searching for Evidence of Correlated Photons Formed by 4-Wave Mixing	PL
Kitchens, Carolyn A.	Appalachian State University	Preparation and Characterization of Proteins and Hybrid Lipid Bilayers on Gold Surfaces	CSTL
Lauterbach, Debra	Iowa State University	Adding Speech to Text Transcription to a Video Annotation Tool	ITL
Le, Michael V.	University of California, Irvine	Investigating Reliability Characteristics of Medium-Sized Service-Oriented Architectures	ITL
Lee, Constance P.	Northwestern University	Grain Growth and Boundary Migration in Strontium Titanate	MSEL
Lee, Jonathan	University of California, Berkeley	Eliminating Rotational Errors in C-AFM's 6-axis Stage	MEL
Lenkner, Jennifer M.	College of Mount St. Joseph	Development, Fabrication, and Characterization of Novel Electrodes for Use as Cell Based Sensors	EEEL
Lewinger, Claire V.	University of Florida	A Study of the Effect of Fire on Steel Framed Buildings	BFRL
Lin, Stephen	University of Pennsylvania	Thermal Characterization of Microhotplate Devices and Gas-Sensor System-on-a-Chip (SoC)	EEEL
Matthews, Paul William	Coppin State University	Reducing NSRL Overhead: Finding Similar Attributes in Multiple Language Versions of Microsoft Windows' Internet Files	ITL
McGruder, Brenna M.	Mississippi State University	Real-Time Measurements for Cancer Detection Using Telomerase	CSTL
McQuighan, Kelly	Rice University	Automation and Testing of a New Plastic Scintillator Dosimeter for Radioactive Sources Used in Prostate Cancer Brachytherapy	PL
Mesick, Nathan J.	Rensselaer Polytechnic Institute	Diffusion in Nickel-Base Superalloys and Bond Coats	MSEL

Student	University	Talk Title	OU
Milliken, Andrew C.	University of Maryland, College Park	Wireless Telemetry for Fire Research and Fire Service Applications	BFRL
Molino, Van	Princeton University	Markov Chains and MCMC Methods	ITL
Montgomery, Eric J.	University of Maryland, Baltimore County	Exciting Frontiers in Single Photon Counting Detectors	PL
Morales, Miguel A.	University of Puerto Rico, Mayaguez	Phase Diagram of a Gas of Atomic Bosons, Atomic Fermions, and Heteronuclear Molecules	PL
Myers, Kathrine E.	Lebanon Valley College	Dynamic Imaging of Lipid Bilayers on Chemically Modified Surfaces	PL
Naff, Jessica L.	Appalachian State University	Re-creation of Accelerant Burn Patterns on Carpet Using the Fire Dynamics Simulator	BFRL
Nishimoto, Bryan I.	University of California, Irvine	Method Development for the Preparation and Analysis of Polymer Samples Using MALDI-TOF Mass Spectrometry	MSEL
Park, G. Barratt	Davidson College	High-Temperature Unimolecular Isomerization Kinetics of 1,4-Pentadiene	CSTL
Pazos, Ileana Marquez	Barry University	Tenary Phase Diagram of the System Bi_2O_3-Fe_2O_3-Nb_2O_5	MSEL
Perez-Andujar, Angelica	University of Puerto Rico, Mayaguez	Test Report of Radiation Detectors Against the ANSI N42.32, N42.33, N42.34, and N42.35 Standards	PL
Pfefferkorn, Candace	Gettysburg College	Nanotube Formation from Biological Membranes Using Optical Tweezers	PL
Pike, Leah	Washington University in St. Louis	Image Analysis of MEMS-Based Nanopositioning Stages	MEL
Radford, Robert J.	University of California, Santa Barbara	An Exploratory Data Analysis for Plutonium Contamination	PL
Rafferty, Ian P.	St. Mary's College of Maryland	Flame Size vs. Heat Release Rates	BFRL
Reedy, Carmen R.	Radford University	Investigations of Explosive Particles in Simulated Fingerprints	CSTL
Robinson, Jenn	Cornell University	Improving Trapping and Detection of BECs in Optical Lattices	PL
Rodriguez-Rivera, Veronica	University of Puerto Rico, Mayaguez	Phase Behavior of Mixed Lipid Bilayered System	MSEL
Ruggles, Dorea R.	Gustavus Adolphus College	Database-assisted Design for Structures Subjected to Wind Loads	BFRL
Santiago Soto, Maria De Lourdes	Inter American University of Puerto Rico, San German	Advanced Inkjet Printing Technology for Trace Explosive Standards	CSTL
Sarnowska, Karolina A.	Mississippi State University	A Comparison of Contention Resolution Schemes for Optical Burst Switching Networks	ITL
Schwarzkopf, Andrew	Cornell University	Size-Dependent Optical Properties of Gold Nanotubes	PL
Shamay, Eric	California Polytechnic State University	Accessing Modern Real Fuels: Kinetic and Thermodynamic Property Databases	CSTL
Simonds, Brian J.	Illinois Wesleyan University	Creating a Nanocapacitor to Measure the Energetics of Molecules in Self-Assembled Monolayers	EEEL
Skaggs, Alan M.	Southern Methodist University	Cutting Forces in Aluminum Alloys	MEL
Smith, Kellie M.	Mississippi State University	Determination of Folate Vitames in Spinach via Liquid Chromatography Combined with Ultraviolet and Fluorescence Detection	CSTL
Speicher, Paul	University of Virginia	Ionizing Radiation Dosimetry Using Water Calorimetry: The Exciting World of Water Temperature	PL
Stanford, Christopher J.	University of Southern California	Sub-millimeter Absorption Spectroscopy of Water Vapor	PL
Stelzenmuller, Anna	Southern Methodist University	Surface Treatment and Characterization of Ag/AgCl Micro-Reference Electrode Arrays for BioElectronics	EEEL
Stover, Tracy	Murray State University	Compton Suppression for Neutron Activation Analysis Applications at the National Institute of Standards and Technology	CSTL
Svetlik, Stephanie	Pomona College	Nanomechanical Properties of TiO_2/Epoxy Nanocomposites	BFRL
Tan, Wei M.	University of Colorado	Investigation of Carbon Contamination of CD Reference Materials	EEEL
Thrift, Alan A.	University of North Carolina, Charlotte	Mechanical Design of a Uniaxial Load Frame with High Load Capacity	MSEL

Student	University	Talk Title	OU
Tsai, Felicia	Rensselaer Polytechnic Institute	Analysis of a Model Drug Delivery System Using Cluster Secondary Ion Mass Spectrometry (SIMS) and Trace Narcotics Detection Using Ion Mobility Spectrometry (IMS)	CSTL
Villalain-Garcia, Angel L.	University of Puerto Rico	Authentication and Authorization in a Distributed Computer Server	ITL
Walker, David C.	University of Rochester	A Standard Architecture for Naval Training Simulations	MEL
Weatherspoon II, MacArthur	University of Cincinnati	Neutron Spectroscopy	PL
Wells, James E.	Davidson College	The Design and Fabrication of a Thermally Driven Outdoor Sealant Tester	BFRL
Wepasnick, Kevin A.	Franklin and Marshall College	Web-based Databases for Chemical Properties	CSTL
Wiley, Jennifer L.	University of Maryland, College Park	Validation Experiments for the Fire Dynamics Simulator, Version 4.0	BFRL
Zeitoun, Ramsey	University of Maryland, College Park	Development of a Bismuth Filter for the Filter Analyzer Neutron Spectrometer	MSEL